

Ukrainian Conference with International Participation



**«CHEMISTRY, PHYSICS
AND TECHNOLOGY OF SURFACE»**

devoted to the 35th anniversary of the
Chuiko Institute of Surface Chemistry of NAS of Ukraine

and

Workshop

**«NANOSTRUCTURES AND NANOMATERIALS
IN MEDICINE:
CHALLENGES, TASKS AND PERSPECTIVES»**

**26-27 MAY 2021
KYIV
UKRAINE**



National Academy of Sciences of Ukraine
Chemistry Division
Chuiko Institute of Surface Chemistry
Scientific Council

"Chemistry and Technology of Surface Modification"
Public organization "Association "Carbon" in Ukraine"
Interbranch Scientific and Technical Complex "Surface Chemistry"

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Book of abstracts

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Матеріали Всеукраїнської конференції з міжнародною участю «Хімія, фізика і технологія поверхні», присвяченої 35-річчю з дня заснування Інституту хімії поверхні ім. О.О. Чуйка НАН України, і семінару «Наноструктури і наноматеріали в медицині: виклики, завдання та перспективи» – Київ, 2021. – 236 с.

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Збірник містить тези доповідей, які було представлено на конференції і семінарі. Тематика конференції: теорія хімічної будови та реакційна здатність поверхні твердих тіл; фізико-хімія поверхневих та міжфазних явищ; хімія, фізика та технологія наноматеріалів; медико-біологічні та біохімічні аспекти вивчення наноматеріалів. Тези доповідей подано в авторській редакції.

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Chemistry Division
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Conference Program

May 26, Wednesday

9:00 – 9:45 Registration of participants

10:00 – 10:15 Opening of the Conference at the Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine

Professor V. Gun'ko

Oral Session 1

Chair: *Dr. (Chem.) I. Laguta*

10:15 – 10:40 V.M. Gun'ko. Quantum-chemically computed integral characteristics of complex nanomaterials (Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).

10:40 – 10:55 Group Photo

10:55 – 11:10 Coffee break

Oral Session 2

Chair: *Dr. (Chem.) M. Borysenko*

11:10 – 11:30 O. Linnik. Nitrogen and metal ions co-modified semiconductive films based on titania in ecological photocatalysis (Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).

11:30 – 11:50 P.I. Kyriienko¹, O.V. Larina¹, D.Yu. Balakin², A.O. Stetsuk², Y.M. Nychiporuk³. Catalytic properties of ZnO/MgO-SiO₂ systems in ETB-process: Effect of composition (¹L.V. Pisarzhevskii Institute of Physical Chemistry, NAS of Ukraine, Kyiv, ²Institute of Physics, NAS of Ukraine, Kyiv, ³Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).

11:50– 12:10 V.V. Shvalagin, A.V. Korzhak, S.Ya. Kuchmiy. Simultaneous photocatalytic oxidation of substituted benzyl alcohols and H₂ evolution over crystalline graphitic carbon nitride under visible light (L.V. Pisarzhevskii Institute of Physical Chemistry, NAS of Ukraine, Kyiv).

12:10 – 12:30 I.B. Bychko, A.A. Abakumov, P.E. Strizhak. Catalysis of hydrogenation reactions by carbon nanomaterials and molecular hydrogen (L.V. Pisarzhevskii Institute of Physical Chemistry, NAS of Ukraine, Kyiv).

12:30 – 12:45 A.M. Grinko, A.V. Brichka, O.M. Bakalinska, M.T. Kartel. Catalytic activity of halloysite nanotubes decorated with nanoceria (Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).

12:45 – 13:00 **M. Samsonenko¹**, S. Khalameida¹, B. Charmas², O. Zakutevskyy¹. **Preparation of meso-macroporous SnO₂ via mechanochemical and microwave treatments and study of its physicochemical, sorption and photocatalytic properties** (¹Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv, ²Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland).

13:00 – 14:00 Break

Oral Session 3

Chair: *Dr. (Chem.) O. Kazakova*

14:00 – 14:20 **S.I. Pokutnyi**, N.G. Shkoda. **The splitting of electron states in germanium/silicon nanosystem with germanium quantum dots: Theory** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

14:20 – 14:40 A. Bukaros¹, K. Konkov¹, I. Kononovich², **A. Herega¹**. **Clustering of printed electronic circuits elements: A formal percolation approach** (¹*Odessa Military Academy, Ukraine*, ²*Odessa National Academy of Food Technologies, Ukraine*).

14:40 – 15:00 **A. Levushenko¹**, V. Karpyna¹, O. Khyzhun¹, O. Bykov¹, O. Kolomys², V. Strelchuk², V. Tkach³, V. Baturin⁴, O. Karpenko⁴. **On the properties of highly-doped ZnO:Al,N films grown at oxygen-poor and oxygen-rich conditions** (¹*Frantsevich Institute for Problems of Material Science, NAS of Ukraine, Kyiv*, ²*V.E. Lashkarev Institute of Physics, NAS of Ukraine, Kyiv*, ³*V. Bakul Institute for Superhard Materials, NAS of Ukraine, Kyiv*, ⁴*Institute of Applied Physics, NAS of Ukraine, Sumy*).

15:00 – 15:20 **O.A. Mishchuk**, B.M. Yarmoliuk, Ye.V. Kobylansky. **Cooperative emergence of vaterite and graphene oxide nanoclusters in the calcium-surfactant-nanocarbonate interfaces** (*Scientific and Research Institute “MASMA”, Kyiv, Ukraine*).

15:20 – 15:40 **A. Kyrylchuk¹**, D. Tománek². **Design and computational study of an all-carbon water desalination membrane** (¹*Institute of Organic Chemistry, NAS of Ukraine, Kyiv*, ²*Physics and Astronomy Department, Michigan State University, East Lansing, USA*).

15:40 – 16:00 **S.N. Osmanova¹**, E.H. Ismailov¹, S.A. Agayeva¹, A.N. Azizova¹, N.M. Aliyeva², R.M. Agayeva³. **Phase composition and magnetic properties of nanopowders obtained by processing of Mn(Fe, Co)/Bi/La nitrates mixtures under hydrothermal conditions** (¹*Institute of Catalysis and Inorganic Chemistry, NAS of Azerbaijan, Baku*, ²*Institute of Petrochemical Processes, NAS of Azerbaijan, Baku*, ³*Azerbaijan State Pedagogical University, Baku*).

16:00 – 16:15 **D. Karoblis¹**, A. Zarkov¹, E. Garskaite², K. Mazeika³, D. Baltrunas³, G. Niaura^{4,5}, A. Beganskiene¹, A. Kareiva¹. **Preparation of perovskite-type solid-solutions applying sol-gel synthetic approach** (¹*Institute of Chemistry, Vilnius University, Lithuania*, ²*Wood Science and Engineering, Department of Engineering Sciences and Mathematic, Luleå University of Technology, Skellefteå, Sweden*, ³*Center for Physical Sciences and Technology, Vilnius, Lithuania*, ⁴*Department of Organic Chemistry, Center for Physical Sciences and Technology, Vilnius, Lithuania*, ⁵*Institute of Chemical Physics, Faculty of Physics, Vilnius University, Lithuania*).

16:15 – 16:30 Y.S. Osokin, V.F. Vargalyuk, V.A. Polonskyy. **Synthesis and composition of some copper(I) maleates** (*Oles Honchar Dnipro National University, Ukraine*).

16:30 – 16:45 M. Bondarenko¹, P. Silenko¹, V. Shvalagin², Yu. Solonin¹, N. Gubareni¹, O. Khyzhun¹, N. Yarova¹. **Influence of doping levels in oxygen-doped g-C₃N₄ on its structural and photoluminescence properties** (¹*Frantsevich Institute for Problems of Materials Science, NAS of Ukraine, Kyiv*, ²*L.V. Pisarzhevskii Institute of Physical Chemistry, NAS of Ukraine, Kyiv*).

16:45 – 17:00 Al.D. Zolotarenko¹, M.T. Kartel¹, E.P. Rudakova², An.D. Zolotarenko², N.A. Gavrylyuk¹, Yu.A. Tarasenko¹, A.D. Zolotarenko², D.V. Schur². **3D products from composites based on Al₂O₃ and carbon nanotubes using CJP 3D printing technology** (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*, ²*Frantsevich Institute for Problems of Materials Science, NAS of Ukraine, Kyiv*).

17:00 – 17:15 Coffee break

17:15 – 18:00 Poster session I (1-83)

May 27, Thursday

Oral Session 4

Chair: **Dr. (Chem.) O. Goncharuk**

10:00 – 10:20 V. Nagaichuk^{1,2}, I. Gerashchenko³, R. Chornopyshchuk^{1,2}, O. Nazarchuk^{1,2}, O. Chepliaka¹, K. Stepanyuk¹. **Clinical experience of application of the sorption composition based on nanosilica in treatment of patients with burns** (¹*National Pirogov Memorial Medical University, Vinnytsya, Ukraine*, ²*MNPE “Vinnytsya Regional Clinical Hospital Vinnytsya Regional Council”, Ukraine*, ³*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

10:20 – 10:40 A.A. Viltsaniuk¹, N.M. Rezanova², P.V. Belyaev¹, V.N. Kravchenko¹. **Nanocomposite surgical suture materials, allografts for tissue joining and tissue alloplastic** (¹*National Pirogov Memorial Medical University, Vinnytsia, Ukraine*, ²*Kyiv National University of Technology and Design, Ukraine*).

10:40 – 10:55 E.V. Dikhtiaruk, T.V. Krupska, L.P. Golovkova, A.A. Kravchenko, A.K. Matkovsky, V.M. Gun'ko. **Designing composite cryogels for controlled drug delivery systems** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

10:55 – 11:10 V.V. Paientko. **Formation of solid compositions with mineral filling having a cleansing effect** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

11:10 – 11:20 I. Petrik¹, T. Hryts², A. Eremenko¹, A. Kravchenko¹, A. Rudenko³, M. Malysheva². **Modification of hemostatic powders based on alginate and dispersed silica with Ag and Ag/Cu nanoparticles** (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*, ²*Taras Shevchenko National University of Kyiv, Ukraine*, ³*Institute of Urology, NAMS of Ukraine, Kyiv*).

11:20 – 11:40 Coffee break

Oral Session 5

Chair: **Dr. (Chem.) O. Bakalinska**

11:40 – 11:55 K.V. Voitko¹, O.M. Bakalinska¹, Yu.I. Sementsov¹, Yu.V. Goshovska². Perspectives of the usage of nano-antioxidants for cardiovascular diseases therapy (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, ²Bogomoletz Institute of Physiology, NAS of Ukraine, Kyiv*).

11:55 – 12:15 A. Eremenko¹, I. Petrik¹, Iu. Mukha¹, N. Vityuk¹, A. Rudenko². Peculiarities of synthesis and bactericidal properties of nanosilver in colloids, on the surface of dispersed SiO₂ and in the structure of textiles (mini-review) (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, ²Institute of Urology, NAMS of Ukraine, Kyiv*).

12:15 – 12:35 Y.V. Goshovska¹, K.V. Voitko², Y.P. Korkach¹, O.M. Bakalinska², V.F. Sagach¹. Evaluation of cardioprotective action of nano-antioxidants based on graphene oxide and its nitrogen-containing derivatives (¹*Bogomoletz Institutte of Physiology, NAS of Ukraine, Kyiv, ²Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

12:35 – 12:55 A.N. Kalinkevich¹, O.V. Kalinkevich¹, Ye.I. Zinchenko¹, A.Yu. Karpenko¹, H.Ye. Polozhii¹, S.N. Danilchenko¹, A.M. Sklyar², I. Buchvarov³, L. Angelova⁴, A. Daskalova⁴. Chitosan based nanostructured materials for medicine (¹*Institute of Applied Physics, NAS of Ukraine, Sumy, ²Sumy State Pedagogical University, Ukraine, ³Physics Department, Sofia University “St. Kliment Ohridski”, Bulgaria, ⁴Institute of Electronics, Bulgarian Academy of Sciences, Sofia*).

12:55 – 13:15 V.V. Konovalova, I.S. Kolesnyk, A.F. Burban. Immobilization of calcium pantothenate in water-oil emulsion by the membrane emulsification technique (*Department of Chemistry, National University of Kyiv-Mohyla Academy, Ukraine*).

13:15 – 14:00 Break

Oral Session 6

Chair: **Dr. (Chem.) N. Roik**

14:00 – 14:20 I.A. Kovalchuk. Selective sorption of heavy metals by natural and modified layer silicates (*Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv*).

14:20 – 14:40 O.V. Markitan¹, N.N. Vlasova¹, Y.V. Sheludko². Interaction of cationic dyes with DNA sorbed onto nanocrystalline dioxide titanium and ceria surfaces (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, ²Kukhar Institute of Bioorganic Chemistry and Petrochemistry, NAS of Ukraine, Kyiv*).

14:40 – 15:00 V.V. Tkach^{1,2}, M.V. Kushnir¹, S.C. de Oliveira², L. Vaz dos Reis³, Y.G. Ivanushko⁴, A.O. da Silva⁵, P.I. Yagodynets¹, Z.O. Kormosh⁶, O.V. Luganska⁷. The theoretical description for hydroxyquinol CoO(OH)-assisted electrochemical determination (¹*Chernivtsi National University, Ukraine*, ²*Universidade Federal de Mato Grosso do Sul, Campo Grande, Brazil*, ³*Universidade de Trás-os-Montes e Alto Douro, Vila Real, Portugal*, ⁴*Bukovinian State Medical University, Chernivtsi, Ukraine*, ⁵*Campus Juruti, Universidade Federal do Oeste do Pará, Brazil*, ⁶*East Ukrainian National University, Lutsk, Ukraine*, ⁷*Zaporizhzhia National University, Ukraine*).

15:00 – 15:15 I.M. Trofymchuk, L.A. Belyakova, N.V. Roik. **MCM-41 silicas with oligosaccharide “host” cavities for binding aromatic “guests”** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

15:15 – 15:30 R. Sensoy, B. Kabak, E. Kendüzler. **Biocoal from walnut shell and usage in naproxen removal** (*Burdur Mehmet Akif Ersoy University, Art and Science Faculty, Chemistry Department, Turkey*).

15:30 – 15:45 H. Yankovych¹, M. Elsässer², N. Hüsing², M. Václavíková¹. Composite materials based on TiO₂ and activated carbon for elimination and photodegradation of adsorbable organic halogens (¹*Institute of Geotechnics, Slovak Academy of Sciences, Košice*, ²*Department of Materials Science and Physics, University of Salzburg, Austria*).

15:45 – 16:00 E. Broda¹, A. Gładysz-Płaska¹, E. Skwarek¹, V. Paientko². Adsorption of uranyl ions on the composite hydroxyapatite/white clay (¹*Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland*, ²*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

16:00 – 16:20 Coffee break

16:20 – 17:00 Poster session II (84-169)

17:00 – 17:15 Conference Closing

Poster Presentation

1. Theory of Chemical Structure and Reactivity of Solid Surface

1. **V. Halysh^{1,2}, J.M. Romero Garcia^{3,4}, A.M. Vidal Castro³, E. Castro^{3,4}, T. Kulik², B. Palianytsia², A. Nikolaichuk², M. Kartel².** **The effect of alkaline, acid and steam-explosion pretreatment of walnut shells and apricot seed shells on lignin yield** (¹National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", ²Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, ³Department of Chemical, Environmental and Materials Engineering, Universidad de Jaén, Spain, ⁴Center for Advanced Studies in Energy and Environment (CEAEMA), Universidad de Jaén, Spain).
2. **O.V. Smirnova¹, A.G. Grebenyuk¹, V.V. Lobanov¹, T.A. Khalyavka², M.V. Shapovalova².** **Spatial structure and IR spectral manifestation of tin impurity sites in titanium dioxide** (¹Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, ²Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv).
3. **V.V. Voloshchuk**, G.V. Lisachuk, R.V. Kryvobok, A.V. Zakharov, Ye.V. Chefranov. **Technology of creating ceramic materials based on the system BaO – SrO – Al₂O₃ – SiO₂** (National Technical University "Kharkiv Polytechnic Institute", Ukraine).
4. **V.V. Voloshchuk**, G.V. Lisachuk, R.V. Kryvobok, V.V. Sarai, A.P. Grebeniuk, M.S. Maistat, A.V. Kryvobok. **Study of the influence of ferromagnetic additives on composite ceramics** (National Technical University "Kharkiv Polytechnic Institute", Ukraine).

2. Physical Chemistry of Surface and Interfacial Phenomena

5. **T.V. Afanasieva.** **Interaction of oxygen with the Cr/Si(001) system: QM/MM study** (Institute of Physics, NAS of Ukraine, Kyiv).
6. **D.Yu. Balakin¹, N.L. Suprun¹, L.Yu. Lopandia¹, Yu.M. Nychiporuk².** **Ad(de)sorption dynamics of carbon monooxide from Mo(110) surface** (¹Institute of Physics, NAS of Ukraine, Kyiv, ²Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).
7. **S.D. Balika**, M.Ya. Sushko. **Photon transport in suspensions of nanoparticles: On the effects of the electric double layer** (Department of Theoretical Physics and Astronomy, Odesa I.I. Mechnikov National University, Ukraine).
8. **A.A. Biliuk**, O.Yu. Semchuk, O.O. Havryliuk. **Simulation of optical characteristics of organic solar cells** (Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).
9. **I.V. Bordeniuk**, S.V. Sologub, R.H. Amirov. **Unusual magnetoresistance changes of thin deuterium-covered W(100) plate induced by high-temperature annealing** (Institute of Physics, NAS of Ukraine, Kyiv).
10. **O.V. Boychuk¹, O.V. Kravchenko², K.D. Pershina^{1,2}.** **The impact of graphite component on redox conversion of iron in composite films Fe-C** (¹Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Kyiv, ²Joint Department of Electrochemical Energy Systems, NAS of Ukraine, Kyiv).
11. **E. Broda¹, E. Skwarek¹, V. Paientko², O. Goncharuk².** **Synthesis and selected physicochemical properties of hydroxyapatite and blue clay composite** (¹Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland, ²Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).
12. **M. Chodkowski¹, K. Terpiłowski¹, O. Goncharuk².** **Comparison of the wettability effect on silica coatings after hydrophobization using hexamethyldisilazane** (¹Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of

Chemistry, Maria Curie-Skłodowska University, Lublin, Poland, ²Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).

13. **T. Cubritcaia.** **On the possibility of using diatomites of the Moldavian deposit for the extraction of direct dyes** (*The Institute of Applied Physics, Chisinau, Republic of Moldova*).
14. **M.L. Dekhtyar**¹, V.M. Rozenbaum², I.V. Shapochkina³, L.I. Trakhtenberg⁴. **Reciprocating host-guest Brownian photomotor** (¹*Institute of Organic Chemistry, NAS of Ukraine, Kyiv, ²Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, ³Department of Physics, Belarusian State University, Minsk, ⁴Semenov Federal Research Center of Chemical Physics, Russian Academy of Sciences, Moscow*).
15. **O. Dudarko**¹, N. Kobylinska², A. Gładysz-Płaska³, M. Majdan³, V. Tertykh¹. **Adsorptive removal uranium(VI) from water solutions by natural and chemical modified diatomite** (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, ²Taras Shevchenko National University of Kyiv, Ukraine, ³Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland*).
16. **V.S. Dutka**¹, Ya.P. Kovalskyi¹, G.G. Midiana². **Influence of surface nature of disperse inorganic oxides on the processes of vinyl monomers radical polymerization** (¹*Ivan Franko National University of Lviv, Ukraine, ²Department of Physical-Chemistry of Fossil Fuels of the Institute of Physical-Organic Chemistry and Coal Chemistry named after L.M. Lytvynenko, NAS of Ukraine, Lviv*).
17. **O.I. Gichan.** **Analysis of non-stationary concentration distribution of active and inactive species in a model electrochemical process** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
18. **I. Ginsari**, R. Nastas. **Adaptation of the ABTS⁺ method for the evaluation of carbonaceous adsorbents redox properties** (*Institute of Chemistry, Chisinau, Republic of Moldova*).
19. **V.P. Grankin**, D.V. Grankin. **Heterogeneous recombination of H-atoms on a wide-gap catalyst with metal nanoclusters** (*Pryazovskyi State Technical University, Mariupol, Ukraine*).
20. **O.D. Kochkodan**, T.K. Deneka. **Surface chemistry and adsorption properties of nanoporous carbon obtained by pyrolysis of carbides** (*National University of Life and Environmental Sciences of Ukraine, Kyiv*).
21. **T.Ye. Korochkova**, V.M. Rozenbaum. **Unidirectional rotation in a hindered rotation potential** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
22. A.D. Terets^{1,2}, **T.Ye. Korochkova**², N.G. Shkoda², V.A. Mashira². **Game theory description of Brownian motors govern by dichotomous deterministic and stochastic fluctuations** (¹*Department of Physics, Taras Shevchenko National University of Kyiv, Ukraine, ²Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
23. **T.Ye. Korochkova**¹, V.M. Rozenbaum¹, I.V. Shapochkina², L.I. Trakhtenberg³. **Temperature-frequency motion control for a slightly fluctuating ratchet** (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, ²Department of Physics, Belarusian State University, Minsk, ³Semenov Federal Research Center of Chemical Physics, Russian Academy of Sciences, Moscow*).
24. **L.F. Kosvanchuk**, O.I. Antonenko, T.D. Ignatova, L.O. Vorontsova. **Effect of azoinitiators of methyl methacrylate polymerization on the phase separation at the formation of polyurethane/poly(methyl methacrylate) interpenetrating polymer networks** (*Institute of Macromolecular Chemistry, NAS of Ukraine, Kyiv*).
25. **G.I. Kovtun.** **Interfacial properties of chitosan lactate at the liquid/air interface** (*Institute of Applied Problems of Physics and Biophysics, NAS of Ukraine, Kyiv*).

26. N.V. Efimova¹, **A.P. Krasnopyorova**¹, G.D. Yukhno¹, D.S. Sofronov², A.I. Kozhokar¹. **Synthesis and sorption capacity of lignin modified with nanodispersed iron oxide with respect to radionuclides** (¹V.N. Karazin National University, Kharkiv, Ukraine, ²State Scientific Institution "Institute for Single Crystal", NAS of Ukraine, Kharkiv).
27. K. Kulyk¹, V. Prabhakaran², J. Laskin³, M. Larsson¹, **T. Kulik**⁴. **Reactive-landing of nickel(II) tartatic acid complexes on self-assembly monolayer surfaces for catalytic applications** (¹Stockholm University, AlbaNova University Center, Department of Physics, Sweden, ²Pacific Northwest National Laboratory, Richland, USA, ³Purdue University, West Lafayette, USA, ⁴Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).
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50. **T.S. Antonenko**, A.B. Brik, N.O. Dudchenko, O.A. Vyshnevskyi. **Study of synthetic iron hydroxides by scanning electron microscopy** (*M.P. Semenenko Institute of Geochemistry, Mineralogy and Ore Formation, NAS of Ukraine, Kyiv*).
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55. L.I. Borysenko¹, **M.V. Borysenko**², V.P. Klius¹, S.V. Klius¹. **Regeneration of activated carbon used for glycerin purification** (¹*Institute of Renewable Energy, NAS of Ukraine, Kyiv, ²Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
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66. A.B. Nadtochiy¹, **A.M. Gorb**¹, B.M. Gorelov², S.V. Shulga², O.O. Korotchenkov¹, O.I. Polovina¹. **Thermal properties of graphene-epoxy nanocomposites** (¹*Faculty of Physics, Taras Shevchenko National University of Kyiv, Ukraine, ²Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
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91. **A.P. Kusyak**¹, A.L. Petranovska¹, V.A. Dubok², V.S. Chornyi³, P.P. Gorbyk¹. **Synthesis and properties of antibacterial materials based on bioactive glass 60S** (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*, ²*Frantsevich Institute of Problems of Materials Science, NAS of Ukraine, Kyiv*, ³*Bogomolets National Medical University, Kyiv, Ukraine*).
92. **P.O. Kuzema**, A.V. Korobeinyk, V.A. Tertykh. **IR spectroscopic study on peculiarities of fumed silica hydridesilylation with triethoxysilane under fluidized bed conditions** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
93. **V.V. Kyshkarova**^{1,2}, I.V. Melnyk^{2,3}. **Silica-based polystyrene-acrylic hybrids as cationic dyes adsorbents** (¹*Technical University of Košice, Slovakia*, ²*Institute of Geotechnics, Slovak Academy of Sciences, Košice*, ³*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
94. **O.M. Lavrynenko**, O.Yu. Pavlenko, M.M. Zahornyi, A.I. Ievtushenko. **Morphology of primary phases used to obtain functional composites based on rare earth oxides doped with silver** (*Frantsevich Institute for Problems of Material Science, NAS of Ukraine, Kyiv*).
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100. **L.V. Nosach¹, E.F. Voronin¹, E.M. Pakhlov¹, O. Sevastyanova², M.E. Lindström².** **Adsorption modifying of nanosilica with lignin in a gaseous dispersion medium** (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, ²KTH-Royal Institute of Technology, Stockholm, Sweden*).
101. **O.I. Oranska¹, Yu.I. Gornikov¹, N.A. Liedienov², V.M. Gun'ko¹.** **On microstructure of nanosized iron oxide (magnetite)** (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, ²Donetsk Institute for Physics and Engineering named after O.O. Galkin, NAS of Ukraine, Kyiv*).
102. **S.F. Taghiyeva¹, S.N. Osmanova², N.M. Aliyeva¹, E.H. Ismailov².** **Acid-base properties of catalysts based on aluminosilicate for hydrogenation of carbon dioxide according to EPR spectroscopy of adsorbed nitroxyl radicals and thermal desorption of adsorbed methanol** (¹*Institute of Petrochemical Processes, NAS of Azerbaijan, Baku, ²Institute of Catalysis and Inorganic Chemistry, NAS of Azerbaijan, Baku*).
103. **Y.A. Onanko¹, D.V. Charnyi¹, S.A. Shevchuk¹, A.P. Onanko², O.P. Dmytrenko², M.P. Kulish², T.M. Pinchuk-Rugal², M.A. Alieksandrov², P.P. Ilyin².** **Optimization of technological parameters of nanocomposites of the multiwalled carbon nanotubes and polyvinyl chloride, polyethylene, porous polystyrene** (¹*Institute of Water Problems and Land Reclamation, NAAS of Ukraine, Kyiv, ²Physics Department, Taras Shevchenko National University of Kyiv, Ukraine*).
104. **M.V. Pasichnyk^{1,2}, M. Vaclavikova², I. Melnyk^{2,3}.** **Textile nanocomposite filters for efficient removal of organic dyes from water** (¹*V.O. Sukhomlynskyi National University of Mykolaiv, Ukraine, ²Institute of Geotechnics, Slovak Academy of Sciences, Košice, ³Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
105. **O.V. Perlova¹, Yu.S. Dzyazko², O.V. Palchik², I.S. Martovyj¹.** **Removal of U(VI) compounds from aqueous solutions using inorganic composites based on amorphous TiO₂ modified with cobalt hexacyanoferrate(II)** (¹*Odesa I.I. Mechnikov National University, Ukraine, ²Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Kyiv*).
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107. **O. Petuhov¹, N. Timbaliuc¹, M. Pascal², T. Lupascu¹.** **Elimination of non-biodegradable components from waters using complex drinking procedures** (¹*Institute of Chemistry, Chisinau, Republic of Moldova, ²Tiraspol State University, Chisinau, Republic of Moldova*).
108. **Yu. Pirskeyy, F. Manilevich, A. Kutsyi, T. Panchyshyn.** **Hydrogen production by catalytic hydrolysis of sodium borohydride using a platinum catalyst** (*Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine, Kyiv*).
109. **E.N. Poddenezhny¹, A.A. Boiko¹, N.E. Drobyshevskaya¹, M.V. Borysenko².** **Biodegradable composite materials based on starch** (¹*Sukhoi Gomel State Technical University, Belarus, ²Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
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112. **A.V. Potapenko**^{1,2}, O.V. Potapenko^{1,2}, M. Zhou². **Atomic layer deposition technique (ALD) for obtaining electrode materials for new generation of LIB** (¹*Joint Department of Electrochemical Energy Systems, NAS of Ukraine, Kyiv, ²Faculty of Materials Metallurgy and Chemistry, Jiangxi University of Science and Technology, Ganzhou, Jiangxi, People's Republic of China*).
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114. **A.V. Redkina**, M.V. Kravchenko, N.D. Konovalova, M.M. Tsyba. **The effect of microwave treatment on the porous structure of zirconium silicate hydrogels** (*Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv*).
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116. **N.I. Romanovska**, P.A. Manoryk, V.M. Grebennikov, O.V. Shulzhenko. **C, S-doped TiO₂ nanostructures: synthesis, structure and photocatalytic activity in antibiotics photodegradation processes** (*L.V. Pysarzhevskii Institute of Physical Chemistry, NAS of Ukraine, Kyiv*).
117. **A.O. Romansky**, V.L. Karbiskii, L.I. Karbivska, V.V. Zaika. **Quantum-mechanical study of Cu, Ag and Au slabs** (*Department of Nanostructures Physics, G.V. Kurdyumov Institute for Metal Physics, NAS of Ukraine, Kyiv*).
118. **L.P. Rudakova**, D.V. Schur. **Features of the formation of a deposit in the arc synthesis of fullerenes** (*Frantsevich Institute for Problems of Materials Science, NAS of Ukraine, Kyiv*).
119. **O.V. Sachuk**¹, V.A. Zazhigalov¹, O.V. Kiziun¹, L.S. Kuznetsova¹, S.N. Shcherbakov², L.Yo. Kotynska¹. **Synthesis of BaO/ZrO₂ nanocomposites by nontraditional methods** (¹*Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv, ²M.G. Kholodny Institute of Botany, NAS of Ukraine, Kyiv*).
120. **O.Y. Sapelnikova**, L.A. Karachevtseva, O.O. Lytvynenko, O.Y. Stronska. **Photoluminescence model in macroporous silicon structures with SiO₂ nano-covering and CdS nanoparticles** (*V.E. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, Kyiv*).
121. **A.V. Semchenko**¹, V.V. Sidsky¹, O.I. Tyulenkova¹, I.Ya. Sulym², M.V. Borysenko². **Synthesis of ZnO nanorods for electronics and solar cells applications** (¹*Advanced Materials Research Laboratory, Francisk Skorina Gomel State University, Belarus, ²Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
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123. **O.V. Shyrokov**¹, T.F. Lobunets¹, O.V. Chudinovych^{1,2}, A.V. Ragulya¹. **Influence of the rare-earth nitrate solutions concentration on the structure formation of perovskite-type oxide phases** (¹*Frantsevich Institute for Problems of Materials Science, NAS of Ukraine, Kyiv, ²National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"*).
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125. **M.Y. Smyrnova-Zamkova**, O.K. Ruban, O.I. Khomenko, O.I. Bykov, O.V. Dudnik. **Effect of heat treatment on the properties and form factor of ZTA powder produced by hydrothermal synthesis in alkaline medium** (*Frantsevich Institute for Problems of Materials Science, NAS of Ukraine, Kyiv*).
126. **H. Starukh**^{1,2,3}, P. Praus^{1,2}. **Synthesis of g-C₃N₄ supported ultrasmall silver nanoparticles for the application in photocatalysis** (¹*Center for Energy and Environmental Technologies, VŠB-Technical University of Ostrava, Ostrava-Poruba, Czech Republic*, ²*Faculty of Materials Science and Technology, VŠB-Technical University of Ostrava, Ostrava-Poruba, Czech Republic*, ³*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
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129. **T.V. Travinskaya**, O.N. Brykova, N.V. Babkina, Ye.P. Mamunya, L.P. Robota, Yu.V. Savelyev. **Structural peculiarities, thermal and viscoelastic properties of ionomeric polyurethanes based on renewable raw materials** (*Institute of Macromolecular Chemistry, NAS of Ukraine, Kyiv*).
130. **G.P. Tsintskaladze**¹, T.M. Sharashenidze¹, L.G. Eprikashvili¹, M.G. Zautashvili¹, M.M. Burjanadze¹, G.G. Iluridze², V.M. Gabunia¹. **New zeolite anionic nanomaterial - preparation and properties** (¹*Petre Melikishvili Institute of Physical and Organic Chemistry, Ivane Javakhishvili Tbilisi State University, Georgia*, ²*LTD AGROHUB, Tbilisi, Georgia*).
131. **V.G. Tsitsishvili**, N.M. Dolaberidze, N.A. Mirdzveli, M.O. Nijaradze, Z.S. Amiridze. **Obtaining of new bactericidal zeolite fillers for papermaking** (*Petre Melikishvili Institute of Physical and Organic Chemistry, Ivane Javakhishvili Tbilisi State University, Georgia*).
132. N.A. Kurgan, V.L. Karbiskii, L.I. Karbivska, **V.V. Zaika**, A.O. Romansky. **Electronic structure of bulk metallic glasses based on iron** (*Department of Nanostructures Physics, G.V. Kurdyumov Institute for Metal Physics, NAS of Ukraine, Kyiv*).
133. **T.B. Zheltonozhskaya**¹, N.M. Permyakova¹, A.S. Fomenko², L.R. Kunitskaya¹, V.V. Klepko¹, L.M. Grishchenko², D.O. Klymchuk³. **Graft copolymer-assisted synthesis of nickel nanoparticles** (¹*Institute of Macromolecular Science, NAS of Ukraine, Kyiv*, ²*Taras Shevchenko National University of Kyiv, Ukraine*, ³*M.G. Kholodniy Institute of Botany, NAS of Ukraine, Kyiv*).
134. **S.O. Zelinskyi**, N.G. Stryzhakova, O.V. Gozhenko, Y.A. Maletin. **Electrochemical impedance spectroscopy as a method to predict and improve the supercapacitor performance** (*Institute for Sorption and Problems of Endoecology, NAS of Ukraine, Kyiv*).

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135. **V.M. Barvinchenko**, N.O. Lipkovska, O.O. Kazakova. **Effect of solvent permittivity on the adsorption of natural polyphenol curcumin on the nanosilica surface** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

136. **L.V. Batyuk**¹, N.N. Kizilova², O.A. Muraveinik³. **Effects of silver nanoparticles *in vitro* on the structural and functional state of RBCs membranes in patients with stomach tumor** (¹*Kharkiv National Medical University, Ukraine*, ²*Warsaw University of Technology, Poland*, ³*Kharkiv City Clinical Hospital No 7, Ukraine*).
137. **V.M. Bogatyrov**¹, M.V. Galaburda¹, M.V. Borysenko¹, B.O. Ivanytska², N.V. Zaimenko². **Influence of metal-containing silica nanocomposites on the growth processes of agricultural plants** (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*, ²*M.M. Gryshko National Botanic Garden, NAS of Ukraine, Kyiv*).
138. **O.G. Bordunova**¹, E.N. Yadgorova¹, H.O. Petrenko¹, R.V. Dolbanosova¹, E.I. Zinchenko², O.V. Kochenko², O.V. Kalinkevich², S.N. Danilchenko², O.G. Astrakhatseva¹, V.D. Chivanov², A.O. Stepanenko³. **Electrochemical method of obtaining nanosized particles of calcium carbonate from eggshells** (¹*Sumy National Agrarian University, Ukraine*, ²*Institute of Applied Physics, NAS of Ukraine, Sumy*, ³*Sumy State University, Ukraine*).
139. **V.D. Chivanov**¹, O.G. Bordunova², E.N. Yadgorova², H.O. Petrenko², R.V. Dolbanosova², O.O. Chekh², O.M. Kalinkevich¹, S.N. Danilchenko¹, Ya.V. Trofimenko¹, V.K. Zaporozhets¹, A.O. Stepanenko³. **TPD-MS method for assessing the degree of dispersion of calcium carbonate particles in composites of the “Calcium Carbonate : Organic Matrix”** (¹*Institute of Applied Physics, NAS of Ukraine, Sumy*, ²*Sumy National Agrarian University, Ukraine*, ³*Sumy State University, Ukraine*).
140. **A.Yu. Chobtarov**, N.V. Chuiko, V.V. Chobtarova, I.K. Kurdish. **Effect of SiO₂ on ATPase activity of *Bacillus subtilis* IMB B-7023** (*Department of Microbiological Processes on Solid Surfaces, D.K. Zabolotny Institute of Microbiology and Virology, NAS of Ukraine, Kyiv*).
141. **A.Yu. Chobtarov**, K.S. Tsyhanenko, Ya.I. Savchuk, L.T. Nakonechna. **Antibiotic activity of silver nanoparticles obtained by green synthesis using different *Penicillium* species** (*D.K. Zabolotny Institute of Microbiology and Virology, NAS of Ukraine, Kyiv*).
142. **A.P. Holovan**, T.V. Krupska, V.V. Turov. **Stimulating film coatings for seeds based on mixtures of silica and biopolymers** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
143. **P.P. Gorbyk**¹, A.L. Petranovska¹, N.M. Korniichuk¹, N.Yu. Lukyanova², V.F. Chekhun². **Antitumor vector systems on the basis of bioactive lectin *Bacillus subtilis* IMB B-7724** (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*, ²*R.E. Kavetsky Institute of Experimental Pathology, Oncology and Radiobiology, NAS of Ukraine, Kyiv*).
144. **L.K. Japaridze**, Ts.S. Gabelia, E.Sh. Salukvadze, N.I. Shalvashvili, N.A. Osipova, T.K. Kvernadze. **Therapeutic and prophylactic drug against anemia of animals** (*Petre Melikishvili Institute of Physical and Organic Chemistry, Ivane Javakhishvili Tbilisi State University, Georgia*).
145. P.P. Gorbyk¹, A.L. Petranovska¹, **N.M. Korniichuk**¹, A.P. Kusyak¹, N.V. Kusyak², N.G. Antonyuk³, O.D. Shcheglov³. **Cisplatin adsorption on the surface of magnetosensitive nanocomposite Fe₃O₄/Al₂O₃/C** (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*, ²*Ivan Franko Zhytomyr State University, Ukraine*, ³*National University of Kyiv-Mohyla Academy, Ukraine*).
146. **R.B. Kozakevych**¹, L.M. Polyshchuk¹, A.V. Tumko², I.M. Furtat², P.V. Vakuliuk², V.A. Tertykh¹. **Polylactide-silica composites for biomedical application with controlled release of active agents** (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*, ²*National University of “Kyiv-Mohyla Academy”, Ukraine*).

147. **A.A. Kravchenko**¹, N.V. Guzenko¹, L.Ya. Shtanova², P.I. Yanchuk², E.M. Pakhlov¹, I.I. Gerashchenko¹, O.V. Goncharuk¹. **Protein adsorption and hemostatic properties of composite materials based on highly dispersed silica and sodium alginate** (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*, ²*Institute of High Technologies, Taras Shevchenko National University of Kyiv, Ukraine*).
148. **L.R. Kunitskaya**, T.B. Zheltonozhskaya, V.V. Klepko. **Carrier systems for anticancer drug on the base of double hydrophilic block copolymers** (*Institute of Macromolecular Chemistry, NAS of Ukraine, Kyiv*).
149. **I.V. Laguta**¹, O.N. Stavinskaya¹, P.O. Kuzema¹, I.V. Skorochod², A.O. Roy², I.K. Kurdish². **Antioxidant and antimicrobial properties of composite of caffeic acid with fumed silica** (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*, ²*D.K. Zabolotny Institute of Microbiology and Virology, NAS of Ukraine, Kyiv*).
150. **O.G. Lomtadze**, G.P. Tsintsikaladze, N.I. Shalvashvili, N.O. Lomtadze. **Clay-sulfur composition against oidium on grapes** (*Petre Melikishvili Institute of Physical and Organic Chemistry, Ivane Javakhishvili Tbilisi State University, Georgia*).
151. **L. Lupascu**, N. Timbaliuc, T. Lupascu. **Antimicrobial activity of the tannins isolated from walnut (*Juglans regia* L.)** (*Institute of Chemistry, Chisinau, Republic of Moldova*).
152. **L. Lupascu**, N. Timbaliuc, T. Lupascu. **Oak tannic compounds and their *in vitro* antimicrobial properties** (*Institute of Chemistry, Chisinau, Republic of Moldova*).
153. **L. Lupaşcu**, O. Petuhov, T. Lupaşcu. **Absorption of *Bacillus cereus* bacteria on activated charcoal obtained from apricot husks** (*Institute of Chemistry, Chisinau, Republic of Moldova*).
154. **O. Nadtocka**, P. Virych, N. Kutsevol, S. Nadtocka. **Hydrogels based on the graft copolymers of chitosan and their sorption-desorption properties** (*Taras Shevchenko National University of Kyiv, Ukraine*).
155. E.F. Voronin, L.P. Golovkova, **L.V. Nosach**. **The effect of the izoelectric point values of the gelatin on its adsorption onto nanosilica surface at various pH** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).
156. **I. Petrik**¹, A. Eremenko¹, S. Rybalko², V. Tretyak², D. Starosyla², O. Deryabin², A. Rudenko³. **Properties of textile materials modified with Ag and Ag/Cu nanoparticles and their virucidal activity in transmission coronavirus model of pigs** (¹*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*, ²*Institute of Urology, NAMS of Ukraine, Kyiv*, ³*SI "L.V. Gromashevsky Institute of Epidemiology and Infectious Diseases NAMS of Ukraine"*, *Kyiv*).
157. **N.M. Permyakova**¹, T.B. Zheltonozhskaya¹, V.I. Karpovsky², R.V. Postoy², V.V. Maksin², S.V. Partsevskaya³, L.N. Grishchenko³, D.O. Klymchuk⁴, V.V. Klepko¹. **Compositions of α -tocopheryl acetate with micellar nanocarriers: preparation, controlled drug release and *in vivo* biological activity** (¹*Department of Polymer Physics, Institute of Macromolecular Chemistry, NAS of Ukraine, Kyiv*, ²*Department of Analytical and Bioinorganic Chemistry and Water Quality, National University of Life and Environmental Sciences of Ukraine, Kyiv*, ³*Department of Macromolecular Chemistry, Faculty of Chemistry, Taras Shevchenko National University of Kyiv, Ukraine*, ⁴*Laboratory of Electron Microscopy, M.G. Kholodny Institute of Botany, NAS of Ukraine, Kyiv*).
158. **I.V. Siora**, T.V. Krupska, V.V. Turov. **Methyl silica/gelatin composite system and its sorption properties** (*Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv*).

159. **I.A. Skorochod**¹, U. Erdenetsogt², A.O. Roy¹, I.K. Kurdish¹. **Changing the profile of phenolcarboxylic acids in barley plants at seed treatment with a nanocomposite complex bacterial preparation Azogram** (¹D.K. Zabolotny Institute of Microbiology and Virology, NAS of Ukraine, Kyiv, ²National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute").
160. **A.A. Skuratovska**, E.V. Dukhopelnykov, Iu.N. Bliznyuk, E.G. Bereznyak, N.A. Gladkovskaya. **Doxorubicin release from the surface of iron oxide nanoparticles in the presence of DNA** (O.Ya. Usikov Institute for Radiophysics and Electronics, NAS of Ukraine, Kharkiv).
161. **T.O. Veklich**, O.V. Golden, O.O. Kardash. **Kinetic regularities of the impact of macrocyclic compound calix[4]arene C-956 on plasma membrane calcium pump and Ca²⁺ concentration in unexcited cells of the myometrium** (O.V. Palladin Institute of Biochemistry, NAS of Ukraine, Kyiv).
162. **O.O. Viltsaniuk**. **The place of nanodispersed silica in the treatment of endogenous intoxication in patients with COVID-19 associated pneumonia: New approaches** (National Pirogov Memorial Medical University, Vinnytsia, Ukraine).
163. **L.M. Yakubenko**, T.G. Gruzina, L.S. Rieznichenko, S.M. Dybkova, N.I. Grishchenko, V.I. Podolska. **Influence of copper nanoparticles on the electrosurface and biochemical parameters of bacterial cells** (Ovcharenko Institute of Biocolloidal Chemistry, NAS of Ukraine, Kyiv).
164. **N. Zhorzholiani**, K. Amirkhanashvili, V. Tsitsishvili, A. Sobolev, L. Khmaladze. **Complex forming properties of anesthetics with transition metals** (Petre Melikishvili Institute of Physical and Organic Chemistry, Ivane Javakhishvili Tbilisi State University, Georgia).

5. Nanostructures and Nanomaterials in Medicine: Challenges, Tasks and Perspectives

165. **E.M. Demianenko**, K.V. Voitko, A.M. Grinko, S.V. Zhuravskyi, Yu.I. Sementsov. **Quantum chemical study of the superoxide radical interaction with initial and O, N-modified graphene-like plane** (Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv).
166. **I.S. Kolesnyk**, V.V. Konovalova, A.F. Burban. **Alginate-magnetite nanocomposite hydrogels as drug delivery systems** (National University of Kyiv-Mohyla Academy, Ukraine).
167. **I.S. Kolesnyk**, V.V. Havrysh, V.V. Konovalova, A.F. Burban. **Pickering emulsions stabilized with magnetite nanoparticles** (National University of Kyiv-Mohyla Academy, Ukraine).
168. **O.A. Kondratska**, N.G. Grushka, S.I. Pavlovych, N.O. Krasutska, R.I. Yanchii. **The effect of germanium citrate on the state of the pro- and antioxidant system of the mice liver in LPS-induced endotoxemia** (Bogomoletz Institute of Physiology, NAS of Ukraine, Kyiv).
169. **Ya.A. Stelmakh**, L.A. Krushinskaya. **Modification of implant surfaces with tricalcium phosphate and noble metal nanoparticles by EBPVD** (E.O. Paton Electric Welding Institute, NAS of Ukraine, Kyiv).

Interaction of oxygen with the Cr/Si(001) system: QM/MM study

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Investigations of the interaction of transition metals and oxygen with silicon surface are important for technological applications because the compounds of transition metals with silicon possess unique optical, thermoelectric and mechanical properties and can be used in conventional silicon technologies. Recently, accelerated oxidation of silicon was found in the presence of submonolayer transition metal films on the Si(001) surface at room temperature [1,2].

The interaction of the Cr/Si(001) surface with molecular oxygen were studied with a hybrid quantum mechanical - molecular mechanical (QM/MM) method with embedded clusters - SIMOMM (Surface Integrated Molecular Orbital Molecular Mechanics). All calculations have been carried out using the GAMESS/TINKER interface [3,4].

It was found that the metal atoms are active centres for the adsorption of atomic and molecular oxygen on the Cr/Si(001) surface. Structures with single and double Cr-O bonds, Cr-O-Si bridge bonds and complex Cr-O-Si three-centre bonds are the most stable initial surface products for oxygen adsorption. Oxygen atoms bind to both chromium and silicon atoms, consistent with previous experimental results (AES, EELS) [1,2].

The adsorption of an oxygen atom next to an already adsorbed oxygen atom is energetically favoured over anywhere in an unoxidized area of the Cr/Si(001) surface. Thus, the growth of oxides on the Cr/Si(001) surface in the form of islets is energetically favourable.

Although the ground state of the reactants, Cr/Si(001) clusters and oxygen molecule or atom, is a quintet, the ground states of products are triplets. The dissociation of molecular oxygen on the Cr active centres on the Cr/Si(001) surface is exothermic.

Investigations of Cr active sites on the Si(001) surface provide the additional information needed for understanding the mechanisms of single-site catalysis and ultrathin oxide film formation.

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Nanocomposites materials based on titanium-containing interpenetrating polymer networks

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In recent years the considerable attention has been devoted to polymeric nanocomposites materials based on titanium dioxide and poly(titanium oxide) due to their unique optical properties, which become interesting for nonlinear optical applications.

Titanium-containing interpenetrating polymer networks (Ti-IPNs) based on the cross-linked polyurethane (PU) and Ti-containing copolymer (Ti-CP) based on hydroxyethyl methacrylate (HEMA) and titanium isopropoxide ($\text{Ti}(\text{O}i\text{Pr})_4$) were obtained by simultaneous synthesis. PU/PHEMA ratio in neat and Ti-IPNs was 30/70 and 50/50 wt.%, and molar ratio HEMA/ $\text{Ti}(\text{O}i\text{Pr})_4$ was 16/1, 8/1 and 4/1.

Study by DSC method showed that increase of the $(-\text{TiO}_2-)$ fragments content in IPNs led to essential increase of glass transition temperature (T_g) and the values of increments of heat capacity (ΔC_p) in Ti-CP. In Ti-IPNs on their basis, this effect was less significant. Analysis of the microheterogenic structure of the Ti-IPNs by the SAXS method revealed that the synthesized hybrid systems possessed nanosized regions of heterogeneity. The increase in the content of the Ti-component was accompanied by increase in the overall level of heterogeneity of the titanium-containing nanocomposite materials.

It was demonstrated that titanium-containing interpenetrating polymer networks are optically transparent with the optical transparency coefficient value up to 90-91 % at 650 nm. The reverse visible darkening of Ti-IPNs under UV-irradiation was observed due to the formation of paramagnetic ions of Ti^{3+} as a result of electron transition $\text{Ti}^{4+} + \text{e} \leftrightarrow \text{Ti}^{3+}$.

Evaluation of the use of nanostructured alumina in the removal of certain chemical elements during the process of natural water purification

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One of the promising methods for water purification is the use of highly efficient sorbents with a highly-developed specific surface area and high adsorption properties, including nanostructured alumina (NP Al₂O₃). In the nanostructured state, this sorbent meets all the requirements established for substances used as sorbents, and therefore attracts the attention of researchers.

The aim of this work was to study the sorption properties of nanostructured alumina powders with various structure characteristics in the simulated media using both negatively charged non-metal ions (B³⁻, Si⁴⁻, P³⁻) and positively charged metal ions (Cr³⁺, Cd²⁺, Pb²⁺, Sr²⁺) as a model.

From the existing alumina preparation methods, the authors selected the method of electron beam evaporation with subsequent vapor deposition in vacuum on the surface (EB PVD). The sorption properties of the synthesized nanostructured alumina were evaluated in model solutions prepared from the reference metal and nonmetal standards used in inorganic analysis. The content of metals and non-metals in the solutions after NP Al₂O₃ sorption was determined by optical emission spectrometry with inductively coupled plasma (OES-ICP). Examination of size and shape of structural components was performed using a laser scanning confocal microscope. Statistical data processing was carried out using the methods of variation statistics.

The studies showed that metal sorption depends on the porosity morphology of nanostructured Al₂O₃, while there was no such correlation detected in case of the sorption of non-metals. Nanostructured Al₂O₃ with inter-crystalline porosity and particle size of 20-70 nm demonstrated a high adsorption capacity. The γ-structure of nanostructured alumina powders appeared out to be an important characteristic for the sorption potential. At the same time, the sorption properties depended on the pH of the model medium. In addition, the degree of adsorption depended also on the adsorbate atom or ion radius. Thus, nanostructured aluminum oxide, obtained by EB PVD is able to absorb and retain on the surface both metal and non-metal ions, which makes it a promising material to be used in water purification.

Study of synthetic iron hydroxides by scanning electron microscopy

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The aim of this work was to investigate of the properties of synthesized goethite and lepidocrocite by both scanning electron microscopy and magnetometry data.

Synthetic goethite was created as follows: a solution of iron(III) nitrate in 2 l of water is slowly poured under cooling and intensive stirring into the ammonia solution, then about 8 l of cold water is added to resulting precipitate, intensively stirred, allowed to precipitate and the washing water is poured off. Then a concentrated solution of potassium hydroxide is added to the precipitate, the mixture is left to stand for 3-4 hours and then for 2 hours water vapor (100 °C) is allowed to pass through the mixture. During this time, the precipitate is completely turned into crystalline light-yellow goethite. The synthesis of lepidocrocite was carried out according to the following procedure: 16.68 g of iron(II) sulphate heptahydrate was dissolved in 300 ml of distilled water and 1M sodium hydroxide was added to adjust the pH=6.7-6.9. The solution was incubated at a room temperature accompanying with air blowing through the solution. During the synthesis, 1M sodium hydroxide was gradually added in order to maintain the pH at the required level. After completion of the reaction (color change from greenish-blue to yellow, cessation of pH change), the obtained precipitate was washed with water and dried to constant weight.

Scanning electron microscope JSM-6700F with a field emission was used to determine the morphology and size of goethite and lepidocrocite nanoparticles. The samples were coated with a platinum film of 30 Å in thickness using sputtering method. Operating conditions of imaging were as follows: SE mode, 10 kV accelerating voltage and 160.65 nA beam current. Scanning electron microscopy of synthetic goethite showed that the sample was represented by aggregates consisting of needle-like goethite particles having a length of 300-500 nm and a width of about 100 nm. Synthetic lepidocrocite reveals the common morphology of flattened scales of several hundred nanometers in length and up to 100 nm in width. The magnetic properties of all the original samples were typical of these minerals. Goethite and lepidocrocite had low magnetization due to antiferromagnetic coupling. Therefore, relatively pure minerals with common morphology and magnetic properties represent all of the starting iron oxides' nanoparticles.

Effect of the way of forming interlayer connection in two-layer polyurethane composites on their viscoelastic properties

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The formation of multi-layer polymer composites is one of the ways to create specific materials. For example, multi-layer design results in improved damping properties. It is known, that many engineering characteristics of materials are determined by their viscoelastic properties. In this work, the effect of the way of forming a contact between layers in two-layer polyurethane (PU) composites has been studied.

Various PU (PU-1 and PU-2) with different oligoglycol and diisocyanate components have been used to form two-layer composites. Three types of two-layer composites were designed where the contact between the layers was formed in different ways. For fabrication of Composite 1, a reaction mixture of PU-2 components was poured onto an already formed PU-1 film. For fabrication of Composite 2, on contrary, a reaction mixture of PU-1 components was poured onto film of PU-2. Composite 3 was fabricated by gluing PU-1 and PU-2 films. To compare the level of interfacial interaction between the layers in Composite 1 and Composite 2, the contact angle (θ) between the surface of PU film-substrate and a drop of liquid urethane mixture was measured. It was shown the θ value is due to both different polarities of the substrates and different chemical nature of drops. But in both cases, $\theta < 90^\circ$ and this means that a good adhesion contact is formed between the layers. Optical images demonstrate a sharp boundary between the layers in Composites 1 and 2, and a darkened strip from the glue seam with a width of $\sim 30 \mu\text{m}$ for Composite 3. Dynamic mechanical analysis (DMA) was used for the investigation of viscoelastic properties of initial PUs and two-layer composites. It was found that the difference in glass transition temperatures (T_g) for PU-1 and PU-2 is 30°C . For two-layer Composites 1 to 3 two relaxation maxima on temperature dependences of loss factor ($\tan\delta$) are observed. Two-layer design leads to broadening of the effective damping temperature range (ΔT), but the position of ΔT depends on the way of connection between the layers. The storage modulus (E') is lower for two-layer Composites 1 to 3 compared with the ones calculated for a similar model system PU-1/PU-2_(model), when the additivity principle is applied. This may be due to the destructive effect of internal stresses at the interface between the layers in fabricated two-layer composites.

Ad(de)sorption dynamics of carbon monooxide from Mo(110) surface

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The kinetics of adsorption of carbon monoxide on the Mo(110) surface at different substrate temperatures and kinetic energies of gas molecules has been studied by molecular beam, thermal desorption with mass spectrometry (TPD), and Auger electron spectroscopy methods. The results obtained made it possible to determine the participation of intrinsic and external states in the adsorption mechanism and to determine the distribution function of the activation energy for desorption of CO molecules from the surface.

When studying the kinetics of adsorption, the dependences of the sticking probability S of CO molecules on the Mo(110) surface on the degree of coverage θ were obtained. In particular, the initial sticking probability S_0 (at $\theta \approx 0$) was determined, which increases from 0.47 to 0.83 as the surface temperature decreases from 880 to 78 K. The dependence of the initial sticking coefficient S_0 on the surface temperature indicates that at the initial stage of the process, adsorption occurs with the participation of an intrinsic state above the free adsorption center.

The TPD spectra obtained in the experiment are described by the Polyani-Wigner equation for the 1st order of the desorption reaction and characterize the distribution of the CO coating into α -, β - and γ -phases. At the beginning of the adsorption process, CO molecules fill β -states, which are reflected by peaks in the TPD spectra at temperatures above 920 K. As the degree of CO coverage increases, the peaks in the TPD spectra expand, indicating the existence of a lateral interaction between the adsorbed molecules. At exposures greater than 1.5 L at the β -peak (1130 K) the shoulder is gradually formed (β_2 -peak at ~1000 K), and at subsequent exposure in the TPD spectra there is a low-temperature α -peak with a maximum at ~380 K, which corresponds to the molecular chemisorption of the CO molecule.

It was found that the first monolayer on the surface of Mo(110) is filled without dissociation of CO molecules into a strongly bound chemisorbed β -phase with a binding energy of 2.1 eV and is completely desorbed only at $T_s = 1200$ K. The second layer (α -phase) is formed on the adsorbed CO molecules, forming a bond with the first monolayer with an energy of 0.7 eV and is desorbed at a temperature of 380 K.

Photon transport in suspensions of nanoparticles: On the effects of the electric double layer

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We look into the possible effects of the electric double layer (EDL) on photon transport in suspensions of nanoparticles, and also the conditions favoring detection of them from experimental data for the extinction and transport mean-free-path lengths of photons and the parameter of scattering anisotropy. The analysis is based on our approach [1] developed by combining the multiple scattering theory with the notion of compact groups [2], redefined for optical problems as groups of particles separated by distances much shorter than the wavelength of scattered light in the carrying liquid. From a physicist's point of view, scattering from such groups is single and can be evaluated by applying the methods of generalized function theory. As a result, the scattering intensity is expressed in terms of the effective one-particle polarizability, formed by multiple scattering and correlation effects within compact groups, and the pair correlation function. For concentrated suspensions, our theory's results significantly differ from those predicted by the Mie theory, but adequately fit experimental data [3].

The theoretical expression obtained for the effective one-particle polarizability has a simple analytical structure. This fact makes it possible to efficiently apply the theory to systems of inhomogeneous particles of various nature. In this report, we present the results of quantitative analysis of the above optical parameters for model systems of particles with adjacent layers, in general inhomogeneous; such layers can be associated with the EDLs. Our results reveal that for certain values of their parameters (thickness, dielectric constant, degree of inhomogeneity), the layers can affect the extinction and transport mean-free-path lengths quite noticeably. We also discuss the situations where experimental registration of the EDL's contributions is expected to be successful.

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Effect of solvent permittivity on the adsorption of natural polyphenol curcumin on the nanosilica surface

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Biomedical investigations of curcumin (1,7-bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione), a major bioactive polyphenolic compound of the turmeric, have provided evidence of a wide range of molecular and cellular activities, most related to antiinflammatory, redox reactions and signal transduction. Many health benefits in the therapy of various complex chronic pathologies, such as Alzheimer's disease, Parkinson's disease, multiple sclerosis, epilepsy, cerebral palsy, atherosclerosis, autoimmune, oncological and cardiovascular diseases have been claimed for curcumin.

The aim of the work was to determine the patterns of sorption and spectral changes of curcumin on the surface of nanosilica depending on the composition of water-ethanol media, widely used in the isolation and standardization of biologically active substances.

The study of curcumin adsorption on nanosilica from water-ethanol solutions in wide range of ethanol concentrations (5-96 %) showed that curcumin is not sorbed from solutions with $C_{\text{EtOH}} > 55 \%$. The decrease of ethanol concentrations $< 55 \%$ promotes curcumin adsorption which increases linearly ($r^2 = 0.975$) with the water content in water-ethanol solutions. It was also found a linear correlation between the adsorption values of curcumin and the permittivity of corresponding water-ethanol solutions. The interaction of curcumin with the nanosilica surface in water-ethanol solutions and the effect of the solvent permittivity on the stability of adsorption complexes was also studied by quantum chemistry methods using solvation models.

The adsorption of curcumin on the nanosilica surface is described with the L4-isotherm, which characterizes the transition from monomolecular (at $C_{\text{Curcumin}} < 1.5 \cdot 10^{-4} \text{ M}$) to polymolecular adsorption, when curcumin adsorbs in the form of aggregates, forming in solutions at higher concentrations ($C_{\text{Curcumin}} > 1.5 \cdot 10^{-4} \text{ M}$). The conditional molar absorption coefficient of sorbed curcumin ($\varepsilon^S_{434} = 10555 \text{ g/mole}\cdot\text{cm}$) was first determined. It was found the criterion that allows to distinguish two types of curcumin in the solid phase – adsorbed on nanosilica ($\lambda_{\max} = 432\text{-}434 \text{ nm}$) and precipitated ($\lambda_{\max} = 500 \text{ nm}$).

The found patterns and sorption parameters make it possible to develop practical recommendations for the preparation of nanocomposites based on nanosilica and curcumin.

Effects of silver nanoparticles *in vitro* on the structural and functional state of RBCs membranes in patients with stomach tumor

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Biomedical nano/microparticles must have special specific properties, based on the unique size-dependent, have electrochemical, physical and mechanical activity and be clinically useful. This is important for development methods of drug delivery technologies, interact of nanoparticles with the cell of blood, in particular red blood cells (RBCs) membranes. Nanoparticles must not induce severe adverse effects on RBCs at loadings of membrane cells the drugs of necessary for therapeutic applications. In the literature, there is conflicting information regarding the destructive effect of silver nanoparticles (AgNP) on cell morphology, membrane structure and protective effect [1]. In this work, the investigated of AgNP preparations (diameter $d \sim 100$ nm and $d \sim 35$ nm) on RBCs membranes 5 health donors and 10 oncologic patients with stomach cancer using a test protocol described in Standard Test Method for Analysis of Hemolytic Properties of Nanoparticles [2]. The dispersions were prepared by the method described in [3]. The significance of differences between the control and experimental results was assessed using the Student's t -test. Differences between the compared indicators were considered significant at $p \leq 0.05$. Hemolysis levels for all particle concentrations were significantly different from the control of donors. Based on the results obtained, it can be concluded that AgNP penetrate into the RBCs of blood of cancer patients 60 % ($d \sim 100$ nm) and 38 % ($d \sim 35$ nm) more actively, where they probably interact with hemoglobin molecules. Probably, the cytotoxic effect of silver on the erythrocyte membranes of cancer patients is associated with the processes of increased generation of reactive oxygen species and oxidative stress associated with violations of the structural state of the RBCs membranes in cancer patients.

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Simulation of optical characteristics of organic solar cells

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In our study, we used the organic solar cell (OSC) shown in Fig. 1. By changing the geometric parameters of the elements of the cell and its components, we investigated changes in such characteristics as reflection, absorption and transmission of light. For our calculations, the main elements influencing the change in characteristics are PEDOT:PSS, poly(3-hexylthiophene) (P3HT):[6,6]phenyl-C₆₁butyric acid methyl ester (PCBM) on silver nanoparticles. The sizes of silver nanoparticles coincide with the PEDOT layer in which they are located, ie the thickness of the PEDOT layer is 50 nm, the particle diameter is 50 nm, the constant layer of P3HT:PCBM has always remained 100 nm.

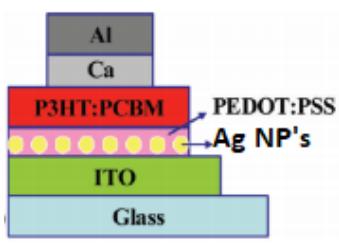


Fig. 1. Architecture of the OSC incorporating Ag nanoparticles in the PEDOT:PSS layer

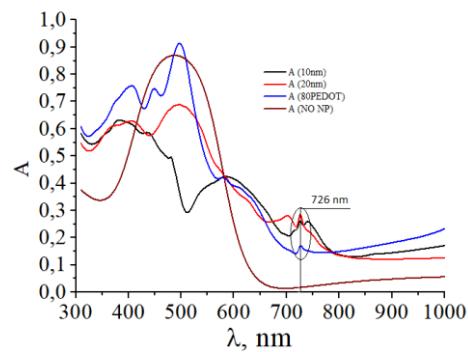


Fig. 2. Absorption spectra of OSC

Fig. 2 shows the absorption spectra of such a solar cell where the curves are responsible for a system where there is 10 nm of free space between the particles, 20 nm of free space, 10 nm of free space when the particles from the mountain and below have 15 nm PEDOT, and no silver particles. As can be seen from Fig. 2. the addition of silver particles significantly increased the absorption coefficient at longer wavelengths (from 600 nm). A peak at a wavelength of about 726 nm, when there are silver particles in the solar cell, indicates the presence of localized plasmon resonance (LSPR), which causes a local amplification of the electromagnetic field near the surface of metal nanoparticles. LSPR induced by Ag nanoparticles not only increased the degree of light absorption, but also increased the degree of exciton dissociation. As a result, the photocurrent and the overall efficiency of the device can be significantly improved after using the optical effects of LSPR.

Influence of metal-containing silica nanocomposites on the growth processes of agricultural plants

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Wheat has been the most important agricultural plant on our planet for millennia. Nevertheless, the UN Food Commission called amaranth a plant of the XXI century, which is recognized as a superfood due to its unusually high nutritional value and edibility of all, without exception, its parts: stems, leaves, seeds. The aim of our work was to study the effect of metal-containing silica nanocomposites on the growth processes of wheat and amaranth.

Composite materials were synthesized using fumed silica as a nanoscale matrix to form nanoparticles of iron oxides, potassium, calcium and ammonium salts. The content of each modifier in the silica composite was 0.2 mmol/g SiO₂. The composites were synthesized using one-stage mechanochemical method in a ceramic ball mill and characterized by thermogravimetry and diffuse reflectance IR Fourier transform spectroscopy. The specific surface area was in the range of 160-264 m²/g.

The allelopathic activity of silica nanocomposites on plants development was studied by the method of biological testing (according to Grodzinsky A.M.) [1] on an amaranth test object (*Amaranthus cruentus* L) in petri dishes and displayed as a percentage compared to control (%). All experiments were carried out in three repetitions. The influence of the addition of nanocomposites on the development of the root system of amaranth was: 118 % for pyrogenic silica, and 119-142 % for silica nanocomposites.

In order to study the effect of silica nanocomposites on the growth processes of wheat (height of the aboveground part, length of roots, weight) the Smuglyanka winter wheat (*Triticum aestivum* L.) was selected as a test object (Table).

Table. The effect of additives on wheat germination, %

The height of the aboveground part	The length of the underground part	Total weight of plants
106.0-109.5	153.2-166.1	107.5-143.8

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The new method of nanocrystal $\text{Y}_2\text{O}_3:\text{Eu}$ powders preparation

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The new versions of ultra-dispersed powders of yttrium oxide doped with europium ions (red phosphor) obtained by thermochemical synthesis (combustion) have been studied. $\text{Y}_2\text{O}_3:\text{Eu}^{3+}$ powders were synthesized by combustion method in and the influence of dispersant was investigated [1].

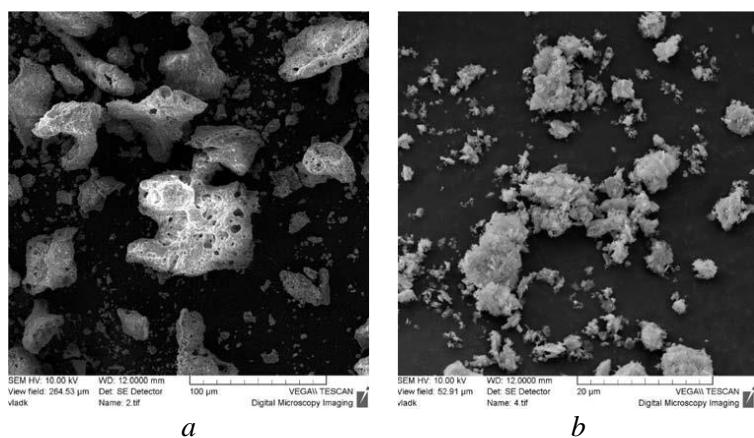


Fig. SEM image of the $\text{Y}_2\text{O}_3:\text{Eu}^{3+}$ samples: *a* – without dispersing agent; *b* – using PVA as dispersing agent

Nanostructured powders of yttrium oxide doped with europium $\text{Y}_2\text{O}_3:\text{Eu}^{3+}$ (red phosphor) were synthesized by the thermochemical method under the conditions of oxidation-reduction of nitrate salts of yttrium and europium in the presence of citric acid as a fuel. The method comprises the following

steps: preparing the starting material, $\text{Y}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ and $\text{Eu}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$; dissolving in citric acid; adding a polyvinyl alcohol (PVA) solution to the mixture to form a precursor; heat stirring and drying the mixture to form a gel-type precursor; and heat treating the precursor to form a nanocrystal $\text{Y}_2\text{O}_3:\text{Eu}^{3+}$ structure. The combustion at the temperature of ignition 350 °C and calcination 650 °C provides removing the PVA and the powders preparation with the average size of coherent scattering region 28–30 nm. The products of powder obtained using polyvinyl alcohol as dispersing agent were characterized by X-ray diffraction, scanning electron microscopy, and IR-spectroscopy.

It was shown that the obtained materials have bright luminescence with a maximum at a wavelength of 612 nm (red radiation) when excited at a wavelength of $\lambda = 393$ nm, and the size of agglomerates and intensity of the radiation depends on the degree of dispersion (Fig.).

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Influence of doping levels in oxygen-doped g-C₃N₄ on its structural and photoluminescence properties

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It is known that carbon nitride luminesces at room temperature, which is promising for light-emitting structures [1]. A comparison of the luminescence bands of the obtained O-doped carbon nitride samples when excited by light with the wavelength (380 nm) is shown in Fig. *a*. As can be seen, the shape of the luminescence bands and the positions of their maxima are close. However, the intensity of the luminescence bands of the obtained samples differs significantly. As the oxygen content in the material is elevated, the PL intensity decreases. With an increase of the amount of oxygen in the sample in addition to the main luminescence band at 450 nm, there is an additional band with a maximum at about 550 nm, that indicating the appearance of an additional route of radiative recombination of photogenerated charges and may be due to the appearance of additional defects in the band gap of the semiconductor. As can be seen from Fig. *b*, in the excitation spectra of the O-g-C₃N₄ samples with a porous lamellar structure (Fig. *c, d*), during registration at the maximum luminescence (450 nm) there are two main peaks (275 and 370 nm), as well as a clear peak (315 nm). Thus, depending on the oxygen content in the sample, the intensity of its maxima and the ratio of intensities in the excitation spectra differ significantly, which indicates the possibility of regulating the energy structure of the samples by changing the amount of oxygen in the sample.

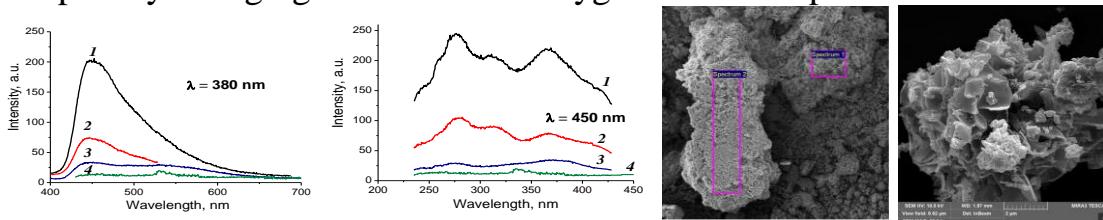


Fig. PL spectra (*a, b*) of samples with oxygen content: 1 – 3%, 2 – 5%, 3 – 7%; 4 – 15%; SEM images (*c, d*) of O-g-C₃N₄ samples

Acknowledgements. This work was supported by research project of NASU “Development of innovative photocatalytic nanostructured materials based on ZnO and TiO₂” (528/IPM-11/20).

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Dependence of photoluminescence properties of O-g-C₃N₄/TiO₂ nanocomposite on the phase composition of the TiO₂ matrix

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In the luminescence excitation spectra during registration at the maximum luminescence (450 nm) of the samples of pure O-g-C₃N₄ and the O-g-C₃N₄/TiO₂ composite (when using the TiO₂ matrix in the form of anatase or rutile, SEM images (Fig. a) of nanoparticles of both composites demonstrate the arrangement of TiO₂ as separate globular nanoparticles and clusters between the plates of the porous scaly plates O-g-C₃N₄) there are two main peaks and a third less clear peak, which indicates the presence of three centers of luminescence excitation in the obtained samples (Fig. b). A comparison of the luminescence bands of the obtained samples of pure O-g-C₃N₄ and the O-g-C₃N₄/TiO₂ composite when excited by light with a wavelength (380 nm) is shown in Fig. c. As can be seen, the shape of the luminescence bands and the position of their maxima are close, however, the intensity of the luminescence bands of the obtained samples differs significantly. The intensity of the photoluminescence bands of the composite samples (especially deposited on the rutile matrix) for 1.5 hours of thermal treatment is significantly lower than the composite samples obtained at short heat treatment time (0.5 h) and pure O-g-C₃N₄. Since luminescence is a process that competes with photochemical transformations, a decrease in the luminescence intensity may indicate the possibility of increased photocatalytic activity of such samples in redox processes.

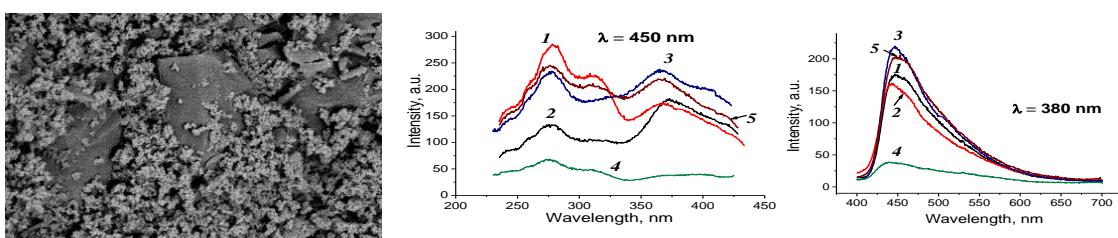


Fig. SEM (a) of O-g C₃N₄/TiO₂-A-1.5h; PL spectra (a, b) of samples: 1 – O-g C₃N₄/TiO₂-A-0.5h, 2 – O-g C₃N₄/TiO₂-A-1.5h, 3 – O-g C₃N₄/TiO₂-R-0.5h, 4 – O-g C₃N₄/TiO₂-R-0.5h, 5 – O-g C₃N₄

Acknowledgements

This work was partially supported by research project of NAS of Ukraine “Development of innovative photocatalytic nanostructured materials based on ZnO and TiO₂” (528/IPM-11/20).

Unusual magnetoresistance changes of thin deuterium-covered W(100) plate induced by high-temperature annealing

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Experimental techniques based on static skin-effect and transversal magnetoresistance [1] were applied for studying of scattering of conduction electrons on surfaces of thin ($100\text{ }\mu\text{m}$) W(100) plates covered up to the saturation by adsorbed deuterium (at $T = 4.2\text{ K}$) and isochronously annealed afterward with increasing and decreasing of temperature. Besides the peculiarities of the plates magnetoresistance (MR) caused by changes in surface scattering specularity induced by deuterium desorption and its submonolayer ordering (Fig., $T = 5 - 800\text{ K}$) [2, 3], unusual, partially reversible MR changes were observed at higher annealing temperatures (Fig., $T = 1250 - 2650\text{ K}$).

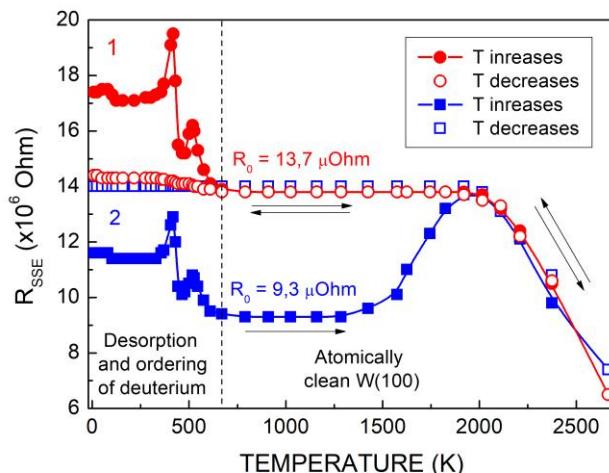


Fig. Change of the MR of the W(100) plate, covered by deuterium at $T \approx 5\text{ K}$, after isochronous ($\approx 1\text{ c}$) annealing. MR-measurements were conducted under static skin effect conditions at $T \approx 5\text{ K}$

Possible reasons for the unexpected high-temperature effect, in particular, the deuterium-induced change of surface and bulk structure of tungsten plates caused by high-temperature “flashes” and penetration of deuterium into the subsurface area of tungsten are discussed.

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Electrochemical method of obtaining nanosized particles of calcium carbonate from eggshells

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This paper presents a simple electrochemical technique for obtaining nanoparticles of calcium carbonate (CaCO_3) from the of bird's eggshells. Aqueous solutions of acetic (peracetic) acid (0.1-10 % v.) were used as the electrolytic liquid. The titanium anode and cathode were placed outside (anode) and inside (cathode) of the half eggshell (Fig.). Electrolytic liquid outside and inside the eggshell half did not mix during electrolysis (2 hours, 60-85 °C). The eggshell undergoes destruction in an acidic medium with the formation of ultra- and nano- dispersed particles. It was shown by TPD-MS method that solid-phase precipitates obtained by drying from an electrolytic liquid inside and outside the shell contain calcium carbonate (CaCO_3) nanoparticles (Fig.). The sample obtained at the cathode (the inner part of the shell) is distinguished by a smaller particle size. This conclusion was made from the fact that a sharp peak of carbon dioxide CO_2 released when calcium carbonate is heated in a vacuum shifts towards low temperatures [1].

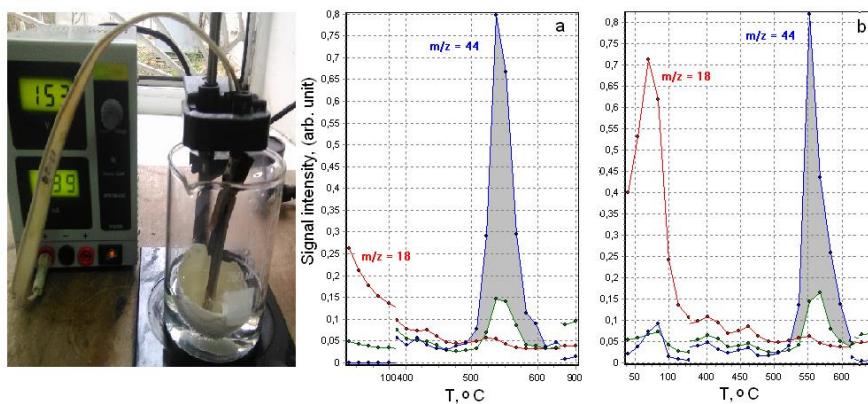


Fig. Electrolysis device (left) and thermogram of electrolytic liquid sediment (1 mg) from the anode space of the electrolytic cell, outer part of the shell (a) and the cathode space, inner part of the shell (b)

Optical properties of Ag₂S quantum dots functionalized with antibodies

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Ag₂S quantum dots are important fluorescent nanomaterials that offer great promise for bioimaging research due to higher photostability, emission intensity and tunable, multicolored emission wavelengths. The surface modification of QD with target biomolecules, such as thiol groups, amino acids, and proteins, is still under exploration. Antibodies are widely used as targeting molecules with QDs for specific cell labelling [1]. The purpose of the study is to functionalize the surface of nanoparticles with antibodies to α -tubulin in plant cells and investigate the changing in their optical properties compared to non-functionalized initial Ag₂S nanoparticles. Bioconjugates with antibodies were prepared using EDC and Sulfo-NHS, which are critical reagents for the covalent coupling process. They create a stable amine-reactive intermediate for binding with antibodies. Luminescence spectra were measured using a Cary Eclipse serial spectrophotometer (Varian Inc., Agilent Tech, USA). It was found that luminescent maxima of Ag₂S nanoparticles functionalized with antibodies corresponded to $\lambda_m \sim 350$ nm (Fig.). While non-functionalized quantum dots have luminescent peaks at the range 420-460 nm, which corresponds to the properties of biologically synthesized nanoparticles [2]. These nanoparticles can be potentially used in various biotechnological approaches.

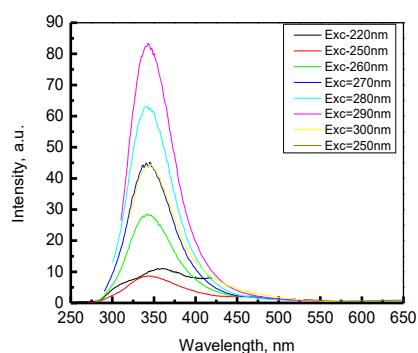


Fig. Luminescent spectra of functionalized Ag₂S quantum dots

1. S.L. Sahoo, C.H. Liu, M. Kumari, W.C. Wu, C.C. Wang. RSC Adv. **9** (2019) 32791.
2. M. Borovaya, A. Naumenko, I. Horiunova, S. Plokhovska, Y. Blume, A. Yemets, Appl. Nanosci. (2020) <https://doi.org/10.1007/s13204-020-01365-3>

Regeneration of activated carbon used for glycerin purification

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Glycerin, the simplest triatomic alcohol $C_3H_5(OH)_3$, is a product of the multi-ton chemical industry. It is used in paints, food, medical, textile, paper, leather, tobacco, agriculture, detergents and cosmetics, plastics such as polyurethanes, glyphthalic, alkyd and epoxy resins. In this work, we investigated granular activated carbons (AC) – initial and spent with adsorbed impurities after purification of technical glycerin. AC was purchased from LLC "Ukrhimresurs", Ukraine. The aim of the study was the regeneration of the spent AC in a combined pyrolysis unit. AC #1 was regenerated at three different modes (samples 1.0, 1.1, 1.2), AC #2 – on two ones (samples 2P, 2T).

Table. Physico-chemical characteristics of the samples

# AC Sample	Specific surface area, m^2/g	Adsorption activity on iodine, %	Mass fraction of moisture, %
1initial	1270	83	0.8
1spent	77	53	14.5
1.0	850	64	0.6
1.1	1090	84	0.5
1.2	740	75	0.9
2initial	1260	92	1.3
2spent	330	48	31.3
2P	1180	58	0.3
2T	610	85	0.3

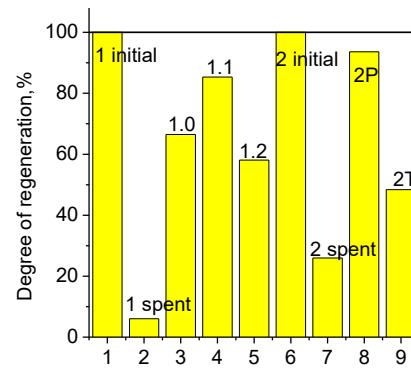


Fig. The degree of AC regeneration, calculated from the values of the specific surface area

It was established by the TGA method that water is released in the temperature range of 20 – 180 °C, and glycerin – 180 – 400 °C. Spent ACs (#1/#2) contain 11.6/29.4 wt.% H_2O and 36.9/6.9 wt.% $C_3H_5(OH)_3$. The combined pyrolysis unit (Institute of Renewable Energy of the National Academy of Sciences of Ukraine, Department of Renewable Organic Energy) has been successfully used for the regeneration of spent activated carbon. As a result, the amount of water (Table) and glycerin in the samples were significantly reduced. The highest degree of regeneration of the samples of AC after activation, calculated from the values of the specific surface area was 85 and 94 % (Fig.).

Adsorption of uranyl ions on the composite hydroxyapatite/white clay

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Uranium is more and more extensively applied as a source of energy and can be potentially used for nuclear weapon production. Due to that fact, the problem of uranium expansion in the environment is the object of research and draw attention many scientists. One of the most effective methods of uranium removal from the wastewater (where uranium is present in a low concentration and occurs mainly in the form of uranyl ion, UO_2^{2+}) is the adsorbent usage. It is important to discover an adsorbent which will be effective, widely available and cheap.

The work discusses properties and ability of U(VI) adsorption on a clay, and nanocomposite clay/Hap (hydroxyapatite) obtained by wet method. The adsorbents were characterized by the mentioned below tests: XRD, XRF, the porosity (nitrogen adsorption-desorption method), zeta potential, surface charge density and sorption of U(VI). It was shown that nanocrystal line composites Hap/white clay can be appropriate adsorbent for removal of uranyl ions. The adsorption depends on temperature and pH of the solution [1].

1. E. Broda, A. Gładysz-Płaska, E. Skwarek, V.V. Payentko, Applied Nanoscience (2021).

Synthesis and selected physicochemical properties of hydroxyapatite and blue clay composite

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Hydroxyapatite (HAP) composites are very important biomaterials, which can be applied in various life areas. HAP composite with blue clay was prepared and studied using X-ray diffraction, nitrogen adsorption, Fourier transform infrared spectroscopy (FTIR), potentiometric titration, and quasi-elastic light scattering and zeta potential measurements. The values of pH_{pzc} (point of zero charge) and pH_{IEP} (isoelectric point) characteristic of the electrical double layer depend strongly on the blue clay addition to HAP.

Comparative studies of hydroxyapatite, blue clay and composite by nitrogen adsorption and FTIR methods showed that in most cases composite has the properties nearly intermediate between hydroxyapatite and blue clay taken for the synthesis; however, certain non-additivity is observed for the characteristics due to precipitation of HAP onto clay particles that changes the HAP formation conditions in comparison to HAP formation alone.

Thus, changes in the condition of the composite preparation allow one to control the characteristics of the final materials.

The impact of graphite component on redox conversion of iron in composite films Fe-C

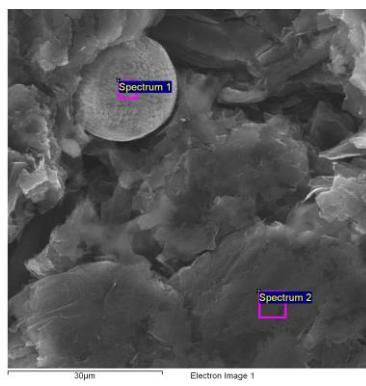
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It is known that the presence of oxides forms the prerequisites for the implementation of several thermochemical reaction surfaces of iron. The final calculations of the main molar enthalpies of iron redox reactions in these systems suggest that the presence of external influence of temperature should lead to a shift in thermodynamic equilibrium and form local zones with the appropriate chemical potential. The presence of carbon and powdered iron in the electrode composition creates thermodynamic prerequisites for the appearance of gradients of electrochemical potential on the electrode surface in the absence of electrical load. The composite films PVDF-Fe-C with a thickness of 200 μm were examined by microprobe analysis of the surface composition (Fig., Table), which showed that the amount of bound oxygen on the surface is more equivalent to the ratios of metal oxides, which may be due to the presence of oxidized graphite. Oxidized graphite is a stronger reducing agent, which should increase the EMF value at a small temperature difference. It was experimentally established that the initial OCV = 7 mV at 10 °C, for 3 hours the heating was carried out at a constant temperature of 30 °C, the maximum OCV = 16 mV, 30 minutes after cessation of heating OCV = 12mV and was constant during the day, confirming the effect of graphite component on thermo-EMF formation.

Table. The surface composition of the composite film, wt.%



Spectrum	C	O	F	Al	Si	Cr	Mn	Fe
Spectrum 1	23,21	48,83		0,14	0,34	0,58	0,67	26,23
Spectrum 2	96,44	2,79	0,77					
Max	96,44	48,83	0,77	0,14	0,34	0,58	0,67	26,23
Min	23,21	2,79	0,77	0,14	0,34	0,58	0,67	26,23

Fig. Areas of spot scanning of the surface

Structure, photoluminescence and photocatalytic activity of ZnO:Co nanostructures

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ZnO nanostructures with different morphology, various optical and electrical characteristics are promising and attractive for photocatalytic processes aimed at both environmental protection and energy activities. The doping of ZnO with transition metals (Fe, Co, Ni, Cu, Mg, Mn) stimulates the growth of photocatalitic activity, presumably by changing the absorption spectrum, reducing the recombination rate of electron-hole pairs when capturing charges on traps. The size of nanoparticles plays a significant role in photoluminescence and photocatalysis.

ZnO:Co nanostructures (NS) with various Co concentrations were grown in tubular furnace with a temperature gradient between substrate place and precursor evaporator place. The process was realized in quasi-closed volume without additional oxygen-argon gas flow. Cobalt acetylacetone powder with various percent ratio (1 to 10 wt.%) to zinc acetylacetone precursor was used as a dopant for growth distinct ZnO:Co NS.

X-ray diffraction analysis of the deposited ZnO:Co NS was performed in theta-2theta Bragg-Brentano configuration using CuKa radiation with $\lambda = 0.1542$ nm by the help of DRON-4 diffractometer. XRD confirmed the formation of a crystalline phase of wurtzite ZnO with the most intense reflexes from plane (100), (002), (101), (110) and (103). The absence of the second phase like CoO, Co and Co₃O₄ indicates that Co mainly incorporate into the ZnO lattice. ZnO:Co nanostructures, grown on Si substrate demonstrate intense UV near band edge emission centered at 374 nm with FWHM 130 meV. There are no peaks in the visible area of the optical spectra, that indicate on absence of oxygen vacancies in ZnO lattice in great amount. The best result of methyl-orange dye decomposing (32 %) was obtained for ZnO NS with 5 % Co.

Acknowledgements

This work was partially supported by the research project of NAS of Ukraine “The development of photocatalytic nanocomposites for viruses inactivation in the air” and was partially supported by the research projects of NAS of Ukraine “Development of innovative photocatalytic nanostructured materials based on ZnO and TiO₂”.

Catalysis of hydrogenation reactions by carbon nanomaterials and molecular hydrogen

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This work is dedicated to determination of the nature of catalytic activity of carbon nanomaterials in the hydrogenation reactions of organic compounds by molecular hydrogen. To achieve this goal such issues as determination of the structure of the adsorption sites of hydrogen and organic compounds, structure of active site, reaction mechanism and influence of the structure of carbon nanomaterials on the kinetics of hydrogenation reactions.

The reaction of ethylene hydrogenation as simple and model gas-phase reaction was used as instrument to establish a parameters of the hydrogenation reactions. The multi-walled carbon nanotubes (CNTs) and reduced graphene oxide (rGO) was used as catalysts. In typical case, reaction was carried in the flow reactor at atmospheric pressure using pure gases (99.9999%). Our experiments indicate that than the ethylene and acetylene hydrogenation rate reaches $2.1 \cdot 10^{-7} \text{ mol} \cdot \text{s}^{-1} \cdot \text{m}^{-2}$ and for CNTs and $8 \cdot 10^{-8} \text{ mol} \cdot \text{s}^{-1} \cdot \text{m}^{-2}$ for rGO.

Additionally catalytic activity of CNTs and rGO was shown in the acetylene hydrogenation and selective hydrogenation of nitrocompounds to corresponding aminocompounds in the liquid phase.

At past decade several studies dedicated to the carbon nanomaterials catalytic activity in the hydrogenation reactions have been reported. It was proposed a few different mechanisms of this reaction. However the structure of catalytic active sites on the surface of the carbon nanomaterials in the hydrogenation reaction is still an open problem. It was shown that H₂ activation can take place at the carbon atom vacancies. A possibility of H₂ activation by frustrated Lewis pairs on the carbons surface has been also discussed. Recently, it has been indicated an activation via the π-π interaction for aromatic compounds.

Our experiments indicate an extremely high stability of CNT in a comparison with the typical hydrogenation catalysts in both, hydrogen-rich and ethylene-rich, atmospheres. This offers new opportunities for the CNT-based catalysts application in the hydrogenation reaction at high temperatures, in particular, under conditions when the metal-containing catalysts deactivate due to the carbonaceous deposits formation.

3D printed nanofilled filter material from polypropylene/copolyamide blend

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The developed new method of production of multi-layered fine-fibrous filter materials (FMs) made of polypropylene/copolyamide (PP/CPA, 20/80 wt.%) blend by 3D printing allows enhancement of the filter abilities and expansion of the application spectrum as compared to that produced by extrusion.

The effect of technological conditions of the process (single-screw or twin-screw extruders, presence/absence of orientational drawing) and zirconia (ZrO_2) nanoparticles (2.5 wt.% of PP) on the properties of FMs is studied. It has been shown the possibility of reducing the diameters of the formed in situ PP microfibrils by using the twin-screw extruder, as well as additional orientation drawing. The effect of nano-additive of ZrO_2 on the morphology of fibrous materials is registered that is an increase in the mass fraction of PP fibers and the reduction of their average size (by 1.4 times compared with the initial blend).

Developed FMs are characterized by high efficiency of air purification from solid particles with a size of 0.3 μm . Application of a twin-screw extruder at the stage of blend compounding or single-screw extruder followed by orientational stretching in the course of strand production provides better results as compared to a FMs prepared from blend obtained using a single-screw extruder. Irrespective of the scheme of production, the cleaning efficiency is enhanced as the number of layers is increased. Precision and the efficiency of filtration with a FMs produced by 3D printing is better of the parameters of a material formed by extrusion.

FMs composed of structural units in the form of PP microfibrils filled with the ZrO_2 nanoparticles is characterized by a substantially higher precision and efficiency. It should be noted that double-layered FMs containing the ZrO_2 nanoparticles are of the same air cleaning efficiency as 4-6 layers' thick filters without a filler (even higher, if the particle size is $> 0.5 \mu m$). In prospect, this fact determines the reduction of material and printing time consumption without a loss of the functional parameters of the product.

TPD-MS method for assessing the degree of dispersion of calcium carbonate particles in composites of the “Calcium Carbonate : Organic Matrix”

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This paper presents the results of studying the composites "CaCO₃ - protein" by the method of temperature-programmed desorption (TPD-MS) [1]. It has been proven experimentally that the location of the carbon dioxide (CO₂) release peak during the thermal destruction of CaCO₃ depends on the isoelectric point (pI) of the protein that is part of the composite. For example, the peak of CO₂ release from the "CaCO₃ - immunoglobulin G (pI 6.4)" composite is located in the 640-650 °C region, and a similar CO₂ peak of the composite "CaCO₃ - cytochrome C (pI 10.7)" is in the 540-550 °C region (Fig.). This is due to both the size of the CaCO₃ particles and their location in the composite.

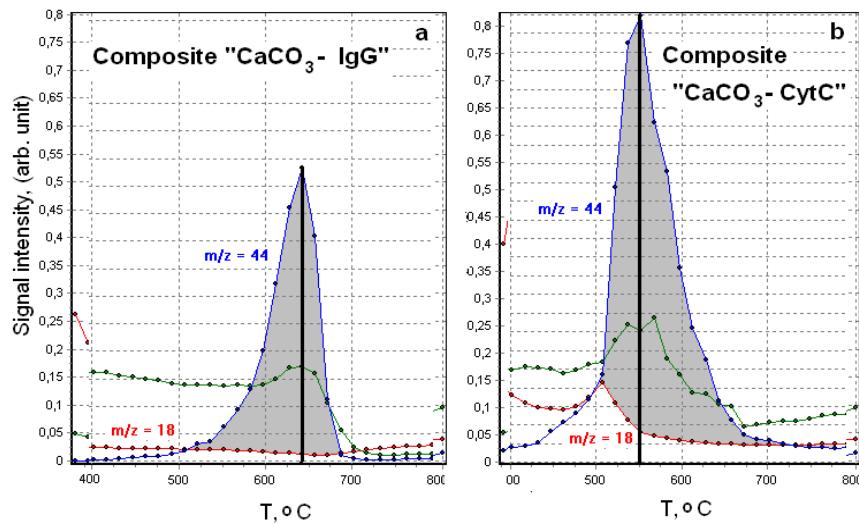


Fig. Thermogram of CO₂ release ($m/z = 44$) by thermal decomposition of sample "CaCO₃ – Immunoglobulin G" (a) and "CaCO₃ – Cytochrome C" (b) composites

1. N. Koga, in. S. Vyazovkin and N. Koga (Eds), Handbook of Thermal Analysis and Calorimetry. Recent Advances, Techniques and Applications, Elsevier B.V., 2018, vol. 6, p.213.

Effect of SiO₂ on ATPase activity of *Bacillus subtilis* IMB B-7023

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The interaction between microorganisms and solid surfaces is a common natural phenomenon. The introduction of solid particles of different nature and degree of dispersiveness into the culture medium for microorganisms may change the direction of physiological and biochemical processes in cells, which in many cases leads to accelerated growth and enzymatic activity of bacteria. The mechanisms of this effect are often unknown. A relevant role is attributed to the surface properties of solid particles.

One of the materials, capable of affecting the functioning of microorganisms, is silicon dioxide nanoparticles. The aim of this work was to investigate the effect of silicon dioxide nanoparticles on the ATPase activity of *Bacillus subtilis* IMB B-7023.

It was established that the ATPase activity of bacilli increased after the introduction of silicon dioxide into the culture medium. For instance, after the introduction of 0.05 g/l of silicon dioxide, the ATPase activity was 111.16 % higher as compared to the control. The highest ATPase activity of *B. subtilis* was registered after the addition of 0.1 g/l silicon dioxide into the glucose-mineral medium. Under these conditions, the level of the ATPase activity of *B. subtilis* was 133.79 % higher as compared to the control. However, after the introduction of 0.5 g/l silicon dioxide there was a slight decrease in the ATPase activity of the culture.

Thus, it was established that the introduction of silicon dioxide nanoparticles into the culture medium promotes the increase in the ATPase activity of *B. subtilis*. The interaction between bacterial cells and nanoparticles is likely to condition the enhanced permeability of cellular walls, which leads to a higher level of substrate penetrating the cell, and thus improving its utilization, activating the system of energy metabolism of the cell.

Antibiotic activity of silver nanoparticles obtained by green synthesis using different *Penicillium* species

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This investigation is part of our laboratory work devoted to obtaining of silver nanoparticles (AgNPs) by green synthesis method and studying of their physical-chemical and biological characteristics. Cell-free fungal extracts for the subsequent production AgNPs were used after the cultivation of three different species of *Penicillium* genus, which are known producers of biologically active metabolites. There were *P. chrysogenum* 3075 (penicillin producer), *P. griseofulvum* 811 (cephalosporin producer), and *P. citrinum* 125 (citrinin producer), and was used silver nitrate solution. The UV-Vis spectrum of the obtained AgNPs solutions were recorded in ~ 420 nm, the morphology and particle sizes investigated by TEM showed various characters. AgNPs obtained by synthesis with the extract after *P. chrysogenum* 3075 cultivation had an amorphous structure, other AgNPs (with the extract after *P. griseofulvum* 811 or *P. citrinum* 125 cultivations) were in the range of 12 – 35 nm.

The main aim of present study was the evaluation of the antibiotic activity of AgNPs obtained by green synthesis using different species of *Penicillium* genus on a set of the pharmacopoeia test strains. We used 4 strains from the collection of reference test culture from the Culture Collection of IMV of the NAS of Ukraine, including *Staphylococcus aureus* ATCC 6538, *Escherichia coli* ATCC 25922, *Bacillus subtilis* ATCC 6633, *Candida albicans* ATCC 10231. The screening was made by agar well diffusion assay. 0.2 mL of AgNPs solution was added per well; cultivation was carried out at 35 ± 2 °C. Diameters of the inhibition growth zones of test cultures were measured after 18 – 24 h. All experiments were performed four times and the average values of four replicates ($p < 0.01$) were used.

Table. Diameters of the inhibition growth zone of test cultures, mm

Species of fungi for AgNP synthesis	<i>S. aureus</i> ATCC 6538	<i>E. coli</i> ATCC 25922	<i>B. subtilis</i> ATCC 6633	<i>C. albicans</i> ATCC 10231
<i>P. citrinum</i> 125	29 ± 2	23 ± 2	25 ± 3	28 ± 4
<i>P. chrysogenum</i> 3075	30 ± 1	17 ± 2	24 ± 1	25 ± 1
<i>P. griseofulvum</i> 811	31 ± 1	17 ± 1	26 ± 1	26 ± 2

The study results showed the equivalent antibiotic activity of obtained AgNPs against all reference test cultures. We have drawn conclusion the ability to production AgNPs with antibiotic activity by green synthesis is a general property of *Penicillium* genus and does not depend on the species were used.

Comparison of the wettability effect on silica coatings after hydrophobization using hexamethyldisilazane

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Silica-based coatings are advantageous in many applications involving surface and material chemistry. They can be obtained using easy and simple sol-gel method, which is rapidly developing methods of surface modification able to produce such materials as for example ceramics, glass and composites as well as hybrid materials, assisted with dip-coating technique.

The aim was to examine degree of hydrophobization by hexamethyldisilazane (HMDS) of silica coatings on glass plates. The coatings were obtained in a sol-gel process by acid-assisted hydrolysis of tetraethoxysilane (TEOS) and they were applied to the glass supports using the dip coating technique. Hydrophobization were made by the saturated vapours of HMDS in a desiccator as well as using bubbler.

It was found that wettability of obtained substrates was characterized by the contact angle above 83 degrees and the effect appears to be permanent – the contact angles do not change significantly in time. Moreover, the surfaces had very low contact angle hysteresis as well as there are differences in wettability of the coatings depends on hydrophobization method.

Clinical experience of application of the sorption composition based on nanosilica in treatment of patients with burns

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The development of effective methods of combating infectious complications remains a priority in the health-care sector and combustiology in particular. Sorption composition for local use, which includes hydrophilic highly dispersed silicon dioxide, hydrophobic polymethylsiloxane, decamethoxine and metronidazole in certain ratio, is considered promising.

Objective: to evaluate the clinical efficacy of topical application of a sorption composition based on nanosilica in the treatment of patients with burns.

42 patients with IIb-III degree burns with an area of 10–30 % of the body surface were divided into 2 groups. Preparation of the patients of main group ($n=20$) for the skin grafting involved treatment of the wound surface with 0.02 % solution of decamethoxine and the studied sorption nanocomposition. Local treatment of the patients in the comparison group ($n = 22$) in the same period was limited by antiseptics. On the 3rd, 7th, and 14th day microbiological and cytological examination of the wound contents and histological study of the structure of injured tissues were performed according to known methods.

Sufficient antimicrobial properties of the suggested sorption nanocomposition, which is not inferior to existing antiseptics in terms of efficiency, were established. The study of the cellular composition of the wound contents and histological structure of injured tissues confirmed the ability of the agent to positively affect the processes of wound cleansing from pathological secretions, necrotic tissues, stimulate the development of granulation tissue and reparative processes in general.

Topical use of the suggested sorption nanocomposite material should be used in the complex treatment of patients with burns at the stage of wound preparation for skin grafting.

On the possibility of using diatomites of the Moldavian deposit for the extraction of direct dyes

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The investigation of the adsorption of various types of dyes (Straight Scarlet, Methylene Blue, Chrysophenine) on the surface of natural D₁ and heat-treated modified diatomite D₂ obtained from the new deposit in the village of Vyshkauts of the Moldavian deposit were performed.

The pH effect of the model solutions, the dye concentration from 50 to 250 mg/g, the contact time and the dose of diatomite with a grain size of ~0.25 mm on the amount of dye adsorption was studied.

The studies were carried out on the model solutions of dyes with different concentrations, in which different doses of diatomite were adjusted from 2.0 to 20 g/l.

Experiments on natural diatomite at the optimal pH value showed that the degree of extraction of Methylene Blue reaches 50-60 % at the diatomite consumption of 2 g/l. An increase in the dose of diatomite to 20 g/l leads to a significant increase in the degree of extraction even at a high concentration of Methylene Blue (250 mg/l). In contrast to Methylene Blue, the maximum degree of extraction (95 % at the diatomite consumption of 20 g/l) in an acidic environment (pH 2-3) was detected for the Direct Scarlet dye.

It was shown that diatomite was not recognized as an effective adsorbent for a solution of Chrysophenin. The adsorption value was only 5 mg/g with an optimal pH < 2 that can be caused by the peculiarities of the geometric structure of the Chrysophenin molecules.

Modification of diatomite by heat treatment improved its adsorption properties to Direct Scarlet and Methylene Blue dyes. The recovery rate of 90-95 % was achieved at lower diatomite consumption (10-12 g/l).

Thus, diatomite D₂ showed good adsorption capacity in relation to the Direct Scarlet and Methylene Blue dyes. The adsorption properties of D₂ samples modified by heat treatment were improved leading to the decrease in the diatomite consumption by 40-50 %.

Adsorption capacity of heat-treated diatomite of various particle size distribution in relation to dyes in a continuous mode at various process conditions (liquid flow rate, loading of the adsorption column, etc.) has been researched.

Assessment of photoactivity of hybrid photocatalyst TiO_2 /diatomite in solar light

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Wastewater treatment from organic pollutions tends more and more to use high-tech methods based on oxidative degradation processes with application of catalytic and photochemical methods. They are known as advanced oxidation processes (AOPs). Among the various AOPs applied in water treatment, heterogeneous photocatalysis with semiconductor is a technique which is carried out under ambient conditions and a possible use of solar irradiation. One of AOPs is the photocatalytic oxidation using TiO_2 as photocatalyst. Titanium dioxide showed itself to be one of the best materials for environmental protection because of its properties. TiO_2 is a cheap, non-toxic, easily obtainable material capable to mineralize a wide range of organic pollutants to harmless compounds. However, the use of titanium dioxide in nanodimensional form is limited by some drawbacks, such as strong tendency to agglomeration, leading to a decrease in its catalytic properties, difficulty in separating of the catalyst after photodegradation. In addition, photocatalysis requires an artificial radiation source. The first disadvantage can be overcome by using a support on which nanoscale titanium dioxide is fixed. An increase in the photoactivity of titanium dioxide in visible, in particular, sunlight, can be achieved by doping it with various atoms and ions.

The aim of this work was to show the ability of a hybrid photocatalyst TiO_2 /diatomite to destroy organic pollutants in an aqueous solution under the influence of solar irradiation. The photocatalyst was obtained by low-temperature hydrolysis of titanium tetrachloride in the presence of diatomite as a substrate. Sensitivity to visible light was provided by doping with nitrogen. Ammonium hydroxide introduced during the synthesis of the photocatalyst was used as a nitrogen precursor.

Adsorption and photocatalytic degradation performance of the composite were assessed using aqueous methylene blue (MB) solution as model pollutant.

It was shown that the degree of photodegradation of MB by the catalyst sample under the influence of natural sunlight was 30 % higher than the removal of the dye by adsorption alone.

This efficiency of the N-doped TiO_2 /diatomite hybrid photocatalyst shows its potential application in cost-effective solar photocatalytic methods for the decomposition of organic pollutants in aqueous media.

Reciprocating host-guest Brownian photomotor

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Molecular nanodevices, especially those converting non-equilibrium fluctuations into directed motion and controlled by light (Brownian photomotors [1]), have been the focus of much recent research attention (see [2] and refs. therein). In the present study, we establish general operating principles for light-driven molecular machines with the different ground- and photoexcited-state potential energies of the Brownian particle in a surrounding force field. The optomechanical relation between the time dependences of the particle excited-state population and its coordinate is described in terms of a theory developed for the laser-pulse controlled reciprocating Brownian photomotor which consists of the guest dye and host cavitand molecules. The self-consistent analytical time dependences of spectroscopic and mechanical variables are derived in the approximation of parabolic potential profiles of the ground and excited states. As shown, the dependence of the average velocity of reciprocating motion on the ultrashort laser pulse period is a nonmonotonic function, with its maximum corresponding to the optimal operating mode of the molecular machine. In the case when the gradual movement of the dye molecule into the cavitand interior increasingly rules out the fluorescence-quenching twisted state, the excited-state decay rate constant of the guest molecule is a decreasing function of its coordinate. As a result, the fluorescence lifetime of the completely cavitand-included dye should significantly increase compared to that of the cavitand-free or partially cavitand-included dye, as is the case in the reported experiments [3].

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Nanocomposites based on polylactide/silver nanoparticles, obtained by thermochemical reduction of Ag⁺ ions by natural or synthetic polymers

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Interest to the investigations of polymeric composites, containing metal nanoparticles, is rapidly growing within the recent years due to their unique physico-chemical, mechanical and biological properties. Formation of metal-containing nanocomposites, involving macromolecular compounds, is a current trend in scientific researches because of their high-potential practical application.

Ag nanoparticles have prominent optical properties, high catalytic, antibacterial and fungicidal activities and this explains an interest to design and production of polymer-metal and hybrid composites, having controllable structure and particles of nano-size level.

During the last decade researches dealing with elaboration of such hybrid materials, including synthesis of Ag-nanoparticles directly in polymers films, are intensively developed.

Peculiarities of the structural organization of the polymer nanocomposites formed via method of thermochemical reduction of Ag⁺ ions in the polymer films like “PLA–AgPalm–polyethyleneimine” “PLA–AgPalm–chitosan” and at temperature interval from 100 to 170 °C have been investigated by WAXS methods.

The optimal parameters of the Ag⁺ ions thermochemical reduction process in the polymer films are determined: temperature $T=160$ °C and reduction time is 5 minutes. It is shown that with increase of heating temperature the nanocomposites crystallinity degree is growing, and at $T>160$ °C this degree sharply decreases due to melting of the crystalline phase of PLA.

It is determined that average size of the Ag nanoparticles in the polymer matrix using PEI as reductant and stabilizer is equal to 6.7 nm and it is varying in a wide range, at the same time, in a matrix with chitosan the average size is found to be 4.2 nm and it is changing in a narrow range.

It is detected that the PLA-Ag-chitosan polymer nanocomposite has much higher antimicrobial activity comparing to the PLA-Ag-PEI nanocomposite against *S. aureus* and *E. coli* strains, and this is attributed to smaller size of the nanoparticles in this nanocomposite.

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Quantum chemical study of the superoxide radical interaction with initial and O, N-modified graphene-like plane

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The development of convenient antioxidants remains challenges and opens new questions concerning the origin of the surface in free radical scavenging activity, mechanism of the reaction, optimal conditions of the reaction proceeding, the influence of different factors (temperature, pressure, solvent), etc. For better understanding, all of these questions DFT method could be employed. Carbon-based nanomaterials may show reactive oxygen species scavenging effects, that based on their properties to generate radical adducts at sp^2 carbon sites, their possibility to transfer of surface electrons or hydrogen donation from functional groups.

For the modeling of the graphene-like plane (GLP) the polycyclic aromatic cluster ($C_{42}H_{16}$) has been chosen. Oxygen atoms were introduced in the graphene plane as hydroxyl, ketone and lactone groups, whereas Nitrogen as quaternary N^+ , amine and nitro groups. The calculations were carried out by DFT method with functional B3LYP and basis set 6-31G(d,p) and dispersion correction by Grimme by means of Firefly 8.2.0 program package. Interaction of the superoxide radical with GLP in aqueous environment was considered as a substitution of the water molecules to superoxide radical on the surface (Fig.).

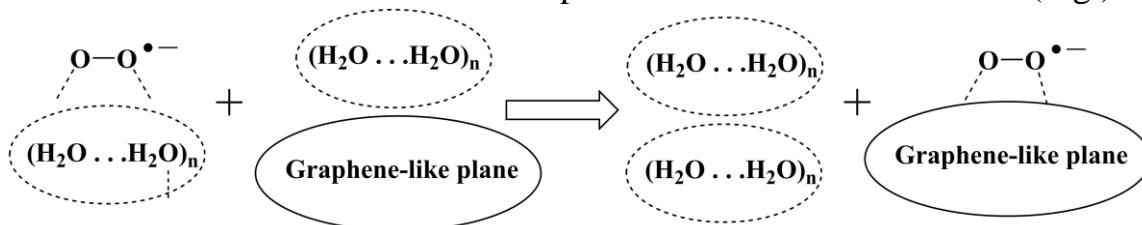


Fig. Modeling of the hydrated superoxide radical interaction with GLP in aqueous solution

Quantum chemical calculations show that the highest interaction energy (- 109.7 kJ / mol) was observed for the GLP with periphery ketone groups. The lowest one – (+ 32.0 kJ / mol) – for the GLP with periphery hydroxyl groups.

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Designing composite cryogels for controlled drug delivery systems

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The unique combination of properties of hydrogels such as biocompatibility, permeability, three-dimensional structure and the ability to swell in water and biological fluids make them promising materials for medicine and have found clinical use. Hydrogels can provide spatial and temporal control over the release of various therapeutic agents, including small-molecule drugs, macromolecular drugs and cells. Owing to their tunable physical properties, controllable degradability and capability to protect labile drugs from degradation, hydrogels serve as a platform on which various physicochemical interactions with the encapsulated drugs occur to control drug release.

The aim of this work was to obtain bioactive composite hydrogels synthesised by cryostructuring and chemical crosslinking based on polyvinyl alcohol (PVA) and chitosan (CS). In this study, we cover mechanisms underlying the design of cryogel drug delivery systems, focusing on physical and chemical properties of the cryogel network and the cryogel–drug interactions across the network. We discuss how different mechanisms interact and can be integrated to exert fine control in time and space overdrug presentation.

The influence of subzero temperatures and the freezing rate on the cryostructuring process has been studied. Composite cryogels on a cotton gauze substrate have been synthesized. Composite cryogels with hydrophilic (A-300) and hydrophobic (AM1) nanosilicas as a carrier with a penicillin antibiotic have been obtained.

As a result of this work, it was shown that by varying cryogelation conditions, which determine the degree of crosslinking and the density of macropore walls, it is possible to prepare the cryogels with a calculated swelling degree. This approach could be used to change the capacity of cryogels as drug (or other bioactive compounds) containers, as well the kinetics of the drug release from their volume. It was shown that matrices based on the PVA/CS cryogel composition have a pronounced hemostatic effect in parenchymal bleeding and are biocompatible.

Properties of nanostructures zinc molybdates synthesized by conventional, hydrothermal and ultrasonic methods

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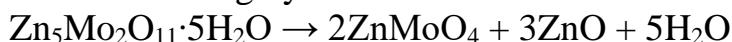
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ZnMoO₄ is a promising material that can be used as material for lithium ion batteries, phosphors for light-emitting diode, anticorrosive paints and *etc.* In this paper, a conventional and several alternative syntheses to create ZnMoO₄ were analyzed.

Conventional co-precipitation synthesis: (NH₄)₆Mo₇O₂₄·4H₂O and Zn(NO₃)₂·6H₂O, in an equimolar ratio of Mo-Zn, were solved in water, with added NH₄OH for precipitation, then added nitric acid for neutral medium. The precipitation was washed several times for removing accompanying ions and dried at 100 °C. XRD analyse showed Zn₅Mo₂O₁₁·5H₂O as single product. The calcinations Zn₅Mo₂O₁₁·5H₂O at 300 °C lead to formation of α -ZnMoO₄ but ZnO was not detecting by XRD:



SEM with EDX confirmed formation two different phases in final product.

MoO₃ and ZnO have been used as raw materials for alternative synthesis that avoid environmental pollution.

Ultrasonic (US) synthesis: MoO₃ and ZnO in water medium was treated ultrasound during 20 minutes at room temperature. X-ray diffraction analysis of product showed the phase ZnMoO₄·0.8H₂O was formed. After calcination at 300 °C it returned into pure phase α -ZnMoO₄. SEM confirmed formation of α -ZnMoO₄ with needle-like structure. The equivalent proportion of metals (Zn-Mo) in the volume of synthesized sample was confirmed by the EDXA.

Barothermal synthesis (BTS): MoO₃ and ZnO in water medium were loaded in teflon-lined stainless steel autoclave and heated at 120 °C for 1 hour. XRD showed the formation ZnMoO₄·0.8H₂O but reflections of initial MoO₃ were presented too. ZnMoO₄·0.8H₂O has needle-like structure (TEM).

Thus, the synthesis of ZnMoO₄ nanostructures from MoO₃ and ZnO as raw materials by alternative methods is very promising, more environmentally friendly, and requires thorough research.

Nanoparticles of solid solutions of gadolinium-yttrium iron garnet: synthesis and magnetic characteristics

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A highly efficient method for the synthesis of nanocrystals of solid solutions of gadolinium-yttrium iron garnet $(Y_{1-x}Gd_x)_3Fe_5O_{12}$ (x - is the mole fraction) was developed and tested. Nanocrystals of solid solutions were synthesized by the method of co-precipitation of hydroxides of yttrium, gadolinium, and iron in boiling water.

Microwave electromagnetic radiation was used to initiate chemical reactions in aqueous precursor solutions, control nucleation, and form new phases. The radiation frequency was 2.45 GHz. We varied the power of electromagnetic radiation from 0.14 to 1.4 kW by changing the duty cycle, i.e., the ratio of the repetition period to the effective pulse duration. The time of the process we changed from 6 to 66 minutes.

It was found that the method used for the synthesis of nanoparticles of solid solutions of gadolinium-yttrium iron garnet provides a powder of a given composition in the form of particles in a shape close to spherical. The mutual solubility of the compounds $Y_3Fe_5O_{12}$ and $Gd_3Fe_5O_{12}$ in the state of solid solutions, the crystal structure, surface morphology, and magnetic properties $(Y_{1-x}Gd_x)_3Fe_5O_{12}$ were investigated.

The average diameter of the obtained particles $(Y_{1-x}Gd_x)_3Fe_5O_{12}$, depending on the magnitude of x and the time of the process, ranged from 20 to 60 nm, the average specific surface area varied from 75 to 25 m^2/g , respectively. Using X-ray analysis, we confirmed the formation of a solid solution phase replacing the garnet structure at $x < 0.2$. The hysteresis loop of the ensembles of dipole-dipole non-interacting nanoparticles of solid solutions $(Y_{1-x}Gd_x)_3Fe_5O_{12}$ was obtained by the method of vibration magnetometry.

We have suggested that the decrease in the specific saturation magnetization of powders obtained by chemical co-precipitation is associated with a decrease in the particle size. The question of the possibility of manufacturing material for solid solutions of gadolinium-yttrium iron garnet with the required magnetic properties by selecting the appropriate composition was discussed.

Adsorptive removal uranium(VI) from water solutions by natural and chemical modified diatomite

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Uranium is one most important element for various industry process, along with the threat to human health and safety due to its high toxicity. This is main reason that uranium contamination is intensively has been studied by numerous researchers. The development of effective methods of water purification requires understanding of nature of uranium compounds (predominantly as UO_2^{2+} ions), their concentration level, etc. The natural diatomite is an abundant and low-cost material compared to other chemically synthesized adsorbents [1]. Also, the surface of diatomaceous earth has the ability for different types of modifications because consist of 85-90 % SiO_2 with active silanol groups, which provide surface functionality promising for the effective and selective removal of contaminants.

In this work was studied the removal U(VI) ions from the aqueous solution by using natural diatomite and its derivative as adsorbents. Natural diatomite (Fig.) was modified with P-containing compounds by different approaches. The effects of the adsorbent modification as well as uranium(VI) adsorption on the diatomite surface have been studied using powder XRD, SEM, N_2 isotherms adsorption/desorption, FTIR spectroscopy, etc.



Fig. Diatomite

Table. Sorption properties of obtained materials towards U(VI) ions

Material	Adsorption (%)
Natural diatomite	6.74
OC-2	91.85
Clay/Vinyl OC-3	77.99
OC-7	95.63

The introduction of phosphonate ligands to the diatomite surface provides effective removal of U(VI) with a high selectivity (Table).

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Influence of surface nature of disperse inorganic oxides on the processes of vinyl monomers radical polymerization

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Dispersion inorganic oxides are introduced into the polymerization systems a significant contribution to the initiation, growth and cliff of polymer chains. In addition, disperse oxide changes the molecular weight and molecular weight distribution of the polymer, which is formed during their presence. Polymer-mineral composite (PMC) may have unique properties and applications for different purposes.

In our work, the results of the study of the adsorption of the components of the polymerization mixture and the peculiarities of formation of polymers in the presence of fine-dispersed mineral oxides are presented. As vinyl monomers used styrene (ST), methyl methacrylate (MMA), methyl acrylate (MA), butyl acrylate (BA) and butyl methacrylate (BMA), and as inorganic oxides – aerosils, PbO, Fe₂O₃, Cr₂O₃, V₂O₅, TiO₂, etc. Peroxide compounds were used to initiate polymerization in homogeneous and filled systems: benzoyl peroxide (BP), oligoperoxide of sebacic acid (OSA) and *tert*-butyl hydroperoxide.

On PbO, Fe₂O₃, Cr₂O₃, V₂O₅ adsorption of BP is also well described by the Langmuir equation. Polymerization of styrene in the presence of aerosil runs out at a lower rate than in the homogeneous system at the same concentration of OSA. This situation is observed with the process with the participation of the Cr₂O₃ surface. In the case of BMA, MMA, MA, a competitive adsorption between monomer molecules and OSA initiator are observed.

The molecular weights of polymers formed in the presence of disperse minerals are usually slightly lower than for polymers obtained in homogeneous conditions. During the polymerization of vinyl monomers, in the presence of disperse minerals there is a grafting of growing polymeric radicals to the surface. The degree of grafting depending on the conditions of polymerization varies widely. In some cases, the method of turbidimetry was determined by the nature of MWD polymers, which are formed in a filled system. The molecular weight distribution of polystyrene is quite wide and in some cases is bimodal. The indicated fact may indicate the role of the surface of mineral oxide to participate in the elementary reaction of the cliff of polymer chains.

Preparation of composite materials in the form of fibers based on polypropylene containing carbon nanofibers with magnetic nanoparticles

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The technology of the preparation of polypropylene (PP) composite fibers containing carbon nanofibers with magnetic nanoparticles have been optimized. The extrusion technique based on the co-melting of the granulated PP and the additive of Fe/C in the weight ratio of 50/50 (content of the additive in the composites was 5.0 w/w %) have been used for the composites' synthesis. The obtained dry strengths were milled to the granules that were further used for the fibers formation using the lab stand. The fiber jet stretch (Φ_B) was 300 and 500 %. The obtained monofibers were exposed to the thermal orientation stretching at 150 °C. The fibers with Φ_B of 300 and 500 % were extended to the stretching degree (λ) equal to 6 and 4, respectively.

Table. Fiber jet stretch and stretching degree of obtained monofibers

Nr.	Sample contents	Φ_B , %	λ
1	PP	300	1
2	PP	300	6
3	PP	500	1
4	PP	500	4
5	PP+5.0 w/w % Fe/C	300	1
6	PP+5.0 w/w % Fe/C	300	6
7	PP+5.0 w/w % Fe/C	500	1
8	PP+5.0 w/w % Fe/C	500	4

As seen, the thermal orientational stretching for composite fibers with the parameters of pure PP was achieved. The higher degree of fibers' breaking during the formation and stretching was observed for the composite samples that can be connected to an inhomogeneous distribution of the additive particles in the polypropylene matrix. It was shown by SEM images that the microfibrillar structure was formed in the case of the composite fibers. The optical microscopy pointed on the inhomogeneous distribution of the additive particles in the polypropylene matrix that can be explained by non-equal stress of loading.

Peculiarities of synthesis and bactericidal properties of nanosilver in colloids, on the surface of dispersed SiO₂ and in the structure of textiles (*mini-review*)

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The purpose of the work is to make a comparative analysis of the biocidal efficiency of AgNPs in the colloidal state, in the structure of dispersed SiO₂ and textile fabrics, depending on the method of synthesis, on the basis of literature data and own researches. The mechanism of action of silver on the microbial cell is the release of silver ions from the surface of the AgNPs into a solution, their adsorption by the protective cell membrane, destruction of membrane proteins, oxidative stress, and destruction of DNA. AgNPs are classified as a safe substance (lethal dose of 5000 mg/kg) but as well as toxic (MPC-50-150 µg/l) with a delayed duration. The efficiency of colloidal AgNPs obtained by green synthesis methods is close to or slightly less than that of NPs obtained by chemical methods and is, depending on the dose (between 2-15 ppm) of silver, 50-80% of bacterial destruction. Extracts of most plants, which exhibit chelating properties, are used as reducing agents. Chemical reduction of ions to the AgNPs (by borohydrides, hydrogen, hydrazine, etc.) allows to regulate the size and shape of the NPs. We found the optimal ratio of NaBH₄ reducing agent and stabilizers of AgNPs with polymer PVP and surfactant SDS, with bactericidal activity of 99 % and stability for more than 3 years. The introduction of AgNPs on the surface of SiO₂ leads to an increase in the time to achieve the required reduction, as well as to changes in the nature of the interaction of NPs with the cells of microorganisms. We have developed effective methods of photochemical synthesis of AgNPs: 1) by irradiation of silver ions in the presence of solid-state photosensitizer SiO₂ with adsorbed benzophenone (BP) molecules - SiO₂/BPads and 2) UV activation of the process of AgNPs formation in the presence of the amino acid tryptophan with clearly defined reaction parameters, which allows the size and properties of the formed particles control. We have also developed a cheap and convenient way to modify textile cotton materials with nanosized silver by soft heat treatment, without stabilizing agents, fiber washing procedures, etc., with high (90 % and above) efficiency of destruction of a number of bacteria *E. coli*, *K. Pneumoniae*, *E. Aerogenes*, *P. Vulgaris*, *S. Aureus*, *C. Albicans*, etc., with preservation of biocidal activity after several cycles of washing, which can be unique and safe for external use.

Quantum chemical modeling of the structure and properties of SnO₂ nanoparticles

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Tin dioxide is one of the classic materials and the research of it is still promising for more than a decade. The wide range of applications of tin dioxide-based materials is due to the combination of a number of unique optical and electrophysical properties. In addition, such materials are non-toxic and cost-effective. The properties of high disperse materials significantly depend on the specific surface area and differ significantly from those of single crystal, so they are paid special attention of researchers. The structure-property relationship may be explained using theoretical modeling methods, in particular quantum chemical ones. In the literature, there are periodic and cluster approaches to modeling the structure and properties of SnO₂. The latter are more convenient for modeling nanoparticles of tin dioxide, because they have no long-range order.

The paper considers molecular models of SnO₂ of different size and composition ($N_{Sn}=1-10$). The results obtained for these models are compared with the experimental data available in the literature. The calculations have been performed by density functional method with exchange-correlation functional B3LYP and basis set 3-21G(d) within the PC GAMESS software package.

From the analysis of the obtained structural parameters of clusters, it follows that the Sn–O bond length does not depend on the cluster size and coordination number for Sn atoms, but depends on the coordination of oxygen atoms (two- or three-coordinated) bound with tin atom. In particular, the length of the Sn–O(III) bond ($\approx 2.10 \text{ \AA}$) is more than that of the Sn–O(II) one ($\approx 1.98 \text{ \AA}$). The calculated Sn–O(III) bond lengths agree well with related experimental values for crystalline SnO₂ (2.05 \AA).

The experimental specific atomization energy of crystalline SnO₂ (1381 kJ/mol) is satisfactorily reproduced (1661 kJ/mol) using the model Sn₁₀H₂₈O₃₄ and related model Sn₂H₈O₈, taking into account the coordination composition of clusters, and water molecules. The theoretically calculated energy gap decreases naturally with increasing cluster size (from 6.14 to 3.46 eV) and approaches the experimental value of the forbidden band gap for the SnO₂ crystal (3.6 eV).

It follows from the above that satisfactory reproduction of the experimental characteristics of crystalline tin dioxide is possible when using clusters containing at least 10 tin atoms.

Photoelectrochemical properties of thin films PbI₂

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In order to analyze the lead content in process fluids and wastewater, it is necessary to develop methods of selective determination concentration of lead ions. Lead is an element that can cause poisoning under adverse conditions. It enters the human body mainly through the respiratory and digestive organs. It is removed from the body very slowly, as a result of which it accumulates in the bones, liver and kidneys [1].

For selective determination of lead, photoelectrochemical analysis of lead accumulation products in the form of lead iodide formed as a result of electrochemical anodic concentration of PbO₂ on transparent conductive SnO₂ electrodes with subsequent conversion to PbI₂ under the HI action is proposed. Photoelectrochemical investigations of PbI₂ thin films have shown that the PbI₂ films in contrast to PbO₂ films have high photosensitivity without the use of annealing.

Analysis of the photoelectrochemical properties of PbI₂ thin films in the wide spectral range of 350–500 nm showed that, depending on the thickness, the quantum efficiency of photocurrent varies. The thickness was controlled by two-beam interferometry [2] during the electrodeposition of PbO₂ at the anode. With increasing thicknesses from 10 to 100 nm, the PbI₂ photocurrent quantum yield increased by linear, then the thickness increases from 100 to 1000 nm it led to decrease. From interferometric studies it was found that with of increasing the concentration of lead in the range of 0.1 mg/l - 1 g/l the PbO₂ film growth was accelerated. The PbO₂ film formation of a 100 nm thick corresponds to a 10-minute anodic concentration with 0.1 mg/l Pb(NO₃)₂ solution and a 1-minute concentration from a 1 g/l Pb(NO₃)₂ solution at 40 mA/cm² current. Thus, the choice of PbO₂ optimal interval of the concentration time allows by the PbI₂ films photocurrent magnitude to determine the lead content within a certain range of concentrations.

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Synthesis and characterization of biochar obtained by pyrolysis of mechanochemical mixture of clay and lignin

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Studies on pyrolytic biochar has gained momentum over activated carbon in the recent years due to its unique properties that are suitable for remediating a range of organic and inorganic contaminants in soil and water environments. The presented work is devoted to the synthesis and study of the structural properties of new functional biochar obtained by pyrolysis of cheap, ecological, renewable and easily accessible raw materials such as lignin, bentonite, and kaolinite.

Biochars were synthesized using two-step method: (i) mechanochemical mixing of kraft lignin (Indulin AT, MeadWestvaco Corp., USA) and clay (bentonite or kaolinite) in a ball mill; (ii) pyrolysis of the mixture in an argon atmosphere at 800 °C. The composites were characterised via XRD, N₂-adsorption/desorption, TGA analysis, and FTIR spectroscopy. It was shown that the synthesized composites are amorphous to X-rays after carbonization and microporous with the specific surface area of 180 m²/g, which is much larger than that of the initial clay. The formation of particles with a spongy texture in bentonite-containing composite and flake type aggregates in the kaolinite-containing composite is observed (Fig.).

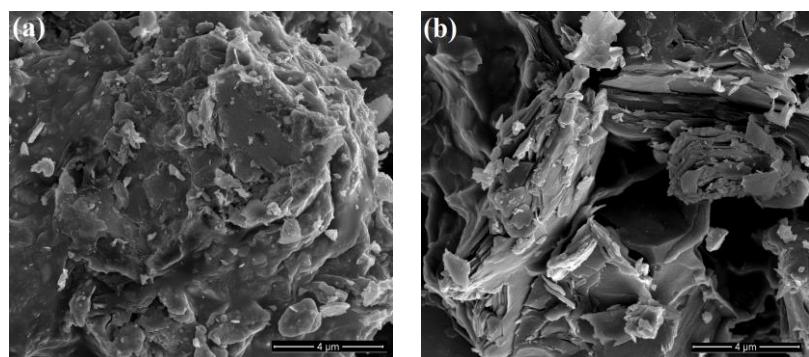


Fig. SEM photos of (a) bentonite- and (b) kaolinite-containing composites

Thus, it is expected that this research will lead to a facile, novel and cost-effective method of obtaining new multifunctional materials, that will be useful in solving problems of environmental protection.

Synthesis and properties of magneto-controlled nanoparticles based on metal ferrites

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Nanoscale materials are a topic of considerable interest across a number of the science, engineering, and biomedical disciplines. The aim of the work was the ability to obtain nickel ferrite magnetic nanoparticles with controllable particle sizes using different approaches and initial reagents.

In this research, nickel ferrite nanoparticles were successfully synthesized through modify sol-gel method using nickel(II) acetate tetrahydrate, iron(III) chloride, and polyethyleneglycol (PEG 1500) in 25 % aqueous solution of ammonia. The final mixture was calcined at 600 °C in an oxidizing air atmosphere.

The as-synthesized NiFe_2O_4 nanoparticles were characterized by means of thermogravimetry, XRD, SEM, FTIR spectroscopy, and vibrating sample magnetometer. According to the XRD data (Fig. a), a cubic phase of nickel ferrite is formed. SEM image demonstrates nanoparticles as tetrahedral and polyhedral pyramids of irregular shapes (Fig. b).

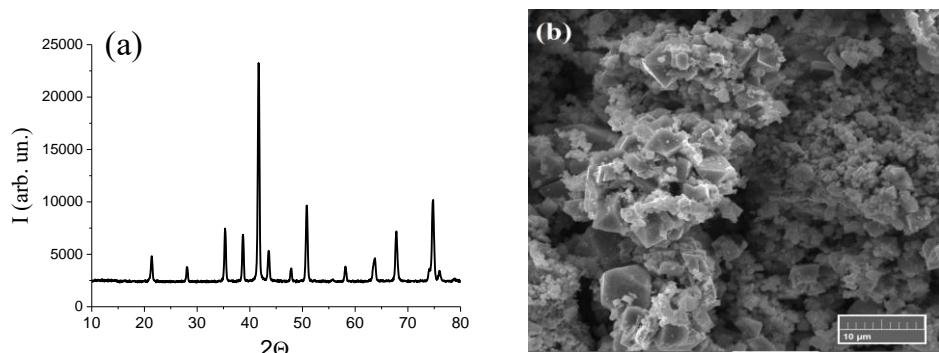


Fig. XRD pattern and SEM image of NiFe_2O_4 nanocomposite calcinated at 600 °C

The proposed method has the advantages of simple preparation and cost-effective route resulting in ultrafine and homogeneous powder that will be used for synthesis of $\text{NiFe}_2\text{O}_4/\text{Ag}$ nanostructures for detection technology in the diagnosis of tuberculosis.

Acknowledgements

This work is carried out within the framework of the NATO project G5798 (A Novel Nanoparticle Based Real-Time Sensor for *B. Anthracis* and *M. Tuberculosis* (NanoSat)). The authors are grateful to the Collective Equipment Center of G.V. Kurdumov Institute for Metal Physics of NASU for the opportunity to use their equipment.

Template directed formation of self-assembling In/InTe nanosystem

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Solid state dewetting (SSD) method as a promising way to obtain nanostructures was applied for the formation of In/InTe nanosystem. The (001) InTe surface is among 2D layered crystals' ones templates suitable for self-assembling of metal nanostructures due to the SSD process. From a physical point of view effective pattern assembly requires nanostructure precursor's mobility over the substrate, a property that is naturally connected with layered crystal surfaces. Due to InTe intrinsic bulk anisotropy its (001) surface might be just easily obtained by cleavage even in UHV thus providing perfect nanosized pattern for obtaining nanosystems with reduced dimension in situ.

The phase-elemental composition and structural perfection of InTe initial surface were characterised by X-ray photoelectron spectroscopy, low energy electron diffraction and atomic force microscopy. X-ray diffraction studies revealed InTe tetragonal crystal structure of the TlSe type (I4/mcm space group, lattice parameters $a = 8.4414(6)$ Å, $c = 7.1333(5)$ Å). Thermal evaporator EFM-3 was applied for In deposition in UHV. Scanning tunneling microscopy (STM) studies of initial (001) InTe surface with ~8 Å parameter square lattice subsequently used as an ordered template in SSD process show that the shape and arrangement of indium induced nanostructures are powered by this lattice symmetry as derived from tetragonal InTe bulk one (Fig.).

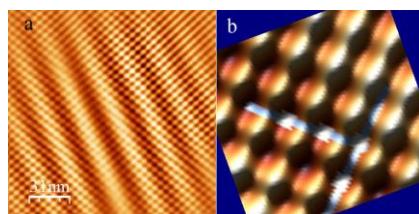


Fig. STM study of In/(001) InTe nanosystem surface: *a*) 2D FFT filtered 153.5×153.5 nm² image after 95 s of In deposition subsequently annealed (200 °C); *b*) 3D zoomed fragment of (*a*)

We observed the formation of nanosized 0D metallic structures in a result of the SSD process due to surface heating above the indium melting point. The scanning tunnelling spectroscopy reveal direct correlation between indium coverage kinetics and increase in the quantity of density of states at the surface within the band gap of InTe.

Analysis of non-stationary concentration distribution of active and inactive species in a model electrochemical process

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This is a theoretical study on analysis of non-stationary concentration distribution of active and inactive species in near-electrode layer in a model electrochemical process with a preceding homogeneous first-order chemical reaction [1, 2]. The impacts of different diffusion coefficients of electrochemically active and inactive species and preceding chemical reaction rate constants on the emergence and development of the concentration patterns is shown (Fig.).

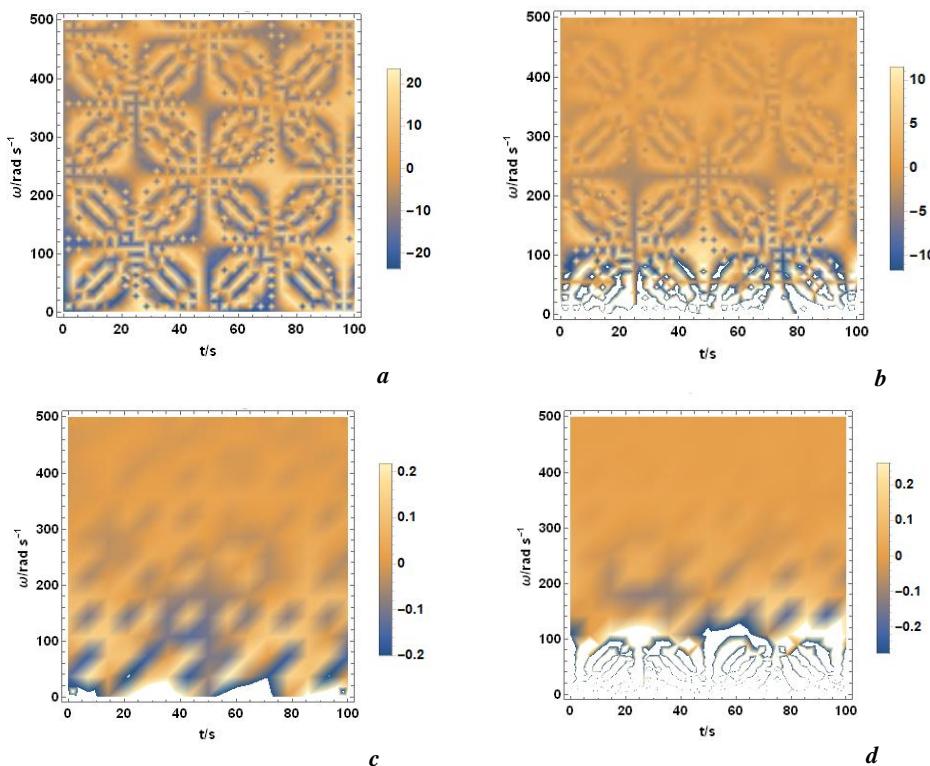


Fig. Deviations of concentrations of electroactive (*a*, *c*) and inactive (*b*, *d*) species from equilibrium concentrations under application of a small amplitude AC. (*a*) and (*b*) – the inner side of the Nernst diffusion layer; (*c*) and (*d*) – the outer side of the Nernst diffusion layer

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Adaptation of the ABTS^{·+} method for the evaluation of carbonaceous adsorbents redox properties

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The most carbonaceous adsorbents applications involve interfacial interactions depending on their surface chemistry, as well as, redox properties. However, the experiments demonstrate that the carbonaceous adsorbents have pronounced catalytic activity in the redox reactions [1, 2]. It was established that the oxygen functional groups, such as hydroxyl, carbonyl or quinone group, are mainly responsible for redox capacity of activated carbons through quinone/hydroquinone redox pair [3]: $> C_xO + H^+ + e \leftrightarrow > C_xOH$.

The purpose of this work was to adapt the ABTS cation radical scavenging method for the evaluation of carbonaceous adsorbents redox properties. The original ABTS^{·+} method is based on the spectrophotometric measurement of ABTS cation-radical (ABTS^{·+}) concentration changes resulting from the ABTS^{·+} reaction with antioxidants [4]. In order to adjust the ABTS^{·+} method for solid samples, different experimental details were considered, including: the activated carbon grain size, solid/liquid ratio, agitation time, total contact time, separation of phases *etc.*

The ABTS^{·+} method for evaluation of the redox properties of activated carbons has been adapted, and the optimal conditions have been established, such as: solid/liquid ratio (0.1÷0.5)/5; contact time 5÷8 min with periodic stirring of 15 sec.; phase separation by filtering with a syringe and recording the absorbance at $\lambda = 734$ nm.

Acknowledgements

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Effect of structural and surface properties of mesoporous TiO₂ on capacitive and cyclic characteristics of composite electrodes of lithium-sulfur batteries

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Sulfur is one of the most high-energy electrode materials investigated for use in lithium power sources. However, its practical application is restricted by significant losses of capacity during cycling and storage, which is due to the solubility of Li_xS_y polysulfides.

The dissolution rate of Li_xS_y depends on the electrolyte composition, nature of the electrically conductive additives, mass characteristics of the electrodes, temperature, and discharge/charge modes. One of the methods allowing for reducing the migration of Li_xS_y from the electrode structure is the use of composite matrices based on nanosized powders of metal oxides. Due to the higher polarity of metal oxides comparing to carbon materials, they are able to absorb Li_xS_y and prevent its migration into an electrolyte. However, the sorption properties of oxides depend both on their composition, structural and surface properties.

The presented work discusses the capacitive and cycling characteristics of TiO₂/S composite cathodes in lithium-sulfur cells. TiO₂/S composites of the mass ratio 3/7 were obtained by impregnation of mesoporous TiO₂ powders with sulfur at the temperature of 130 °C. A method used for the synthesis of TiO₂ and annealing conditions make it possible to obtain nanosized powders differing in structure, particle configuration, specific surface area, pore size, and porosity. It is shown that the impregnation of TiO₂ powders with sulfur significantly changes their morphology, specific surface area, porosity.

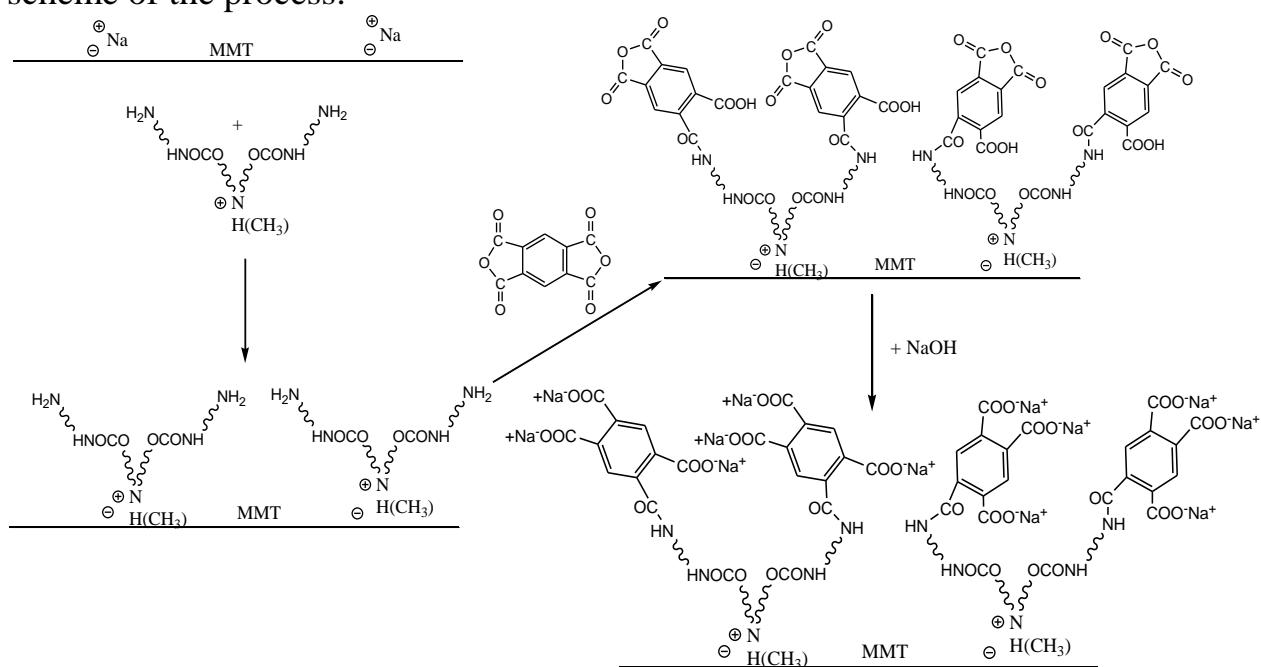
The results obtained in cells using salt-solvate electrolytes show that the capacitive and cyclic characteristics of TiO₂/S composite electrodes depend on the structural and surface properties of TiO₂. Depending on the properties of TiO₂ used in TiO₂/S composite, the specific capacity of sulfur is ~470 mAh/g in the case of rutile TiO₂ and ~600 mAh/g in the case of anatase and brookite TiO₂. Capacity loss for 40 cycles does not exceed 10 % and is minimal for rutile TiO₂.

Functionalization of the montmorillonite surface by carboxylate fragments in order to obtain an aqueous dispersion of organoclay

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Natural inorganic structures such as montmorillonite (MMT) are commonly used to produce polymer nanocomposites. Surface modification of MMT nanoparticles by chemical adsorption of organic cations has opened the opportunities for compatibility of silicate nanoparticles with polymer. The role of the modifier adsorbed on the MMT surface is decisive in the processes of interphase interaction, distribution of nanoparticles in the polymer matrix, the ability to exfoliate the nanofiller. Creating polymer nanocomposites based on specific types of polymers, it is extremely important to develop ways to modify the surface of inorganic particles that will lead to the most efficient realization of the nanofiller. In this work, modified montmorillonite functionalized with hydrophilic compounds was created, which forms aqueous dispersions and can be used to obtain nanocomposites from an aqueous medium based on water-dispersible polymers, in particular ionomeric polyurethanes. To functionalize the surface of montmorillonite with carboxylate fragments, we used the previously modified montmorillonite containing amino groups on its surface [1]. Pyromellitic acid dianhydride was used as a carboxylation agent. General scheme of the process:



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Thermal properties of graphene-epoxy nanocomposites

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Nanostructured graphene-filled polymer composites (G-PNC) are promising candidates for the high-performance thermal-interface materials (TIM) and constitute a rapidly growing research field [1]. From the point of view of industrial application, TIMs based on G-PNCs are attractive because they can be chemically and physically tailored to fulfil specific requirements. As to scientific interest to such TIMs, it is aimed to expose peculiarities of interactions between graphenic materials and polymer macromolecules and to predict their thermal property enhancement versus a level of filler's loading.

For epoxy composites filled with multilayered graphene nanoplatelets (MLG), both thermal conductivity (k_C) and isobaric heat capacity (C_P) have been experimentally and theoretically studied. MLG for experiments have been prepared starting with thermally expanded graphite flakes by using the electrochemical technique [2] followed by an ultrasonic treatment.

Mass fractions (C_f) of MLG varied as 0, 0.5, 1.0, 2.0, and 5 %, k_C has been measured by the well-known 3ω -technique [3], and C_P – by photoacoustic technique [4], at room temperatures. Experimental loading dependences of both k_C and C_P are compared with those calculated by models described in the literature.

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Estimation of interphase layer parameters in polymer nanocomposites by using broad-band dielectric spectroscopy

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In this report we present an experimental approach capable of numerical estimating interphase layers (IPL) characteristics in particulate-filled polymer nanocomposites (PNC), that is based on measuring both dielectric permittivity (ϵ_1) and dielectric loss factor (ϵ_2) of a filler and a polymer matrix.

The experimental studies have been carried out with PNCs based on epoxy and polyester resins filled with oxide nanoparticles, namely silica, titania and silica-titania fumed oxide. The mass fraction of the fillers varied from 0 to 5%. The frequency dependences of complex dielectric permittivity of both the matrices and their nanocomposites have been measured for the frequency range of 10 Hz–5 MHz within the temperature interval of 85–320 K.

Then, the experimental data obtained were compared with theoretical values of calculated from the relations predicted by the so-called interlayer model proposed earlier by Steeman and Maurer [1] to estimate complex dielectric permittivity for a heterogeneous material with an interfacial layer between filler particles and matrix. It should be noted that the model involves so-called the depolarization factor n which can be considered as a measure of filler-matrix interfacial interaction.

By such a comparison, the frequency-averaged values of some IPL' parameters, namely volume fraction, dielectric permittivity and dielectric losses have been estimated. For these estimations, we used required filler's parameters from the literature. Also, the interphase layer thickness has been estimated by using empirical models for IPLs available in literature.

It is shown that differences in IPL' parameters for the different fillers can be treated as coming not only from differences in their intrinsic dielectric properties but also from variations in the n -factor.

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Antitumor vector systems on the basis of bioactive lectin *Bacillus subtilis* IMB B-7724

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In order to create new magneto-sensitive vector systems on the basis of bioactive compounds, a nanobiocomposite (magnetic fluid with adsorbed lectin *B. subtilis* IMB B-772) was synthesised. A methodology of lectin (L) adsorption on the surface of nanoparticles of magnetic fluid (MF) has been developed.

In cooperation with IEPOR after R.E. Kavetsky NAS of Ukraine, the effects of nanobiocomposites on livability and proliferation of cancer cells of a mammary gland of a man MCF-7 in *in vitro* system have been shown. A cell line MCF-7- hormone dependant, adherent cells of mammary adenocarcinoma of a man with epithelial phenotype. The impact of the studied preparations on the amount of live cells MGC of a man is given in a Figure.

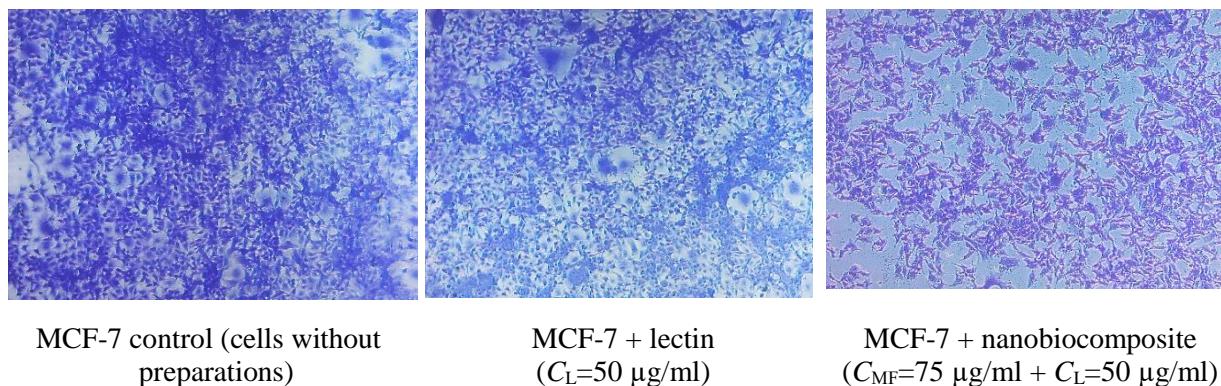


Fig. The impact of the studied preparations on the amount of live cells MGC of a man

The analysis of cytotoxic activity of nanocomposite, lectin and MF showed that nanobiocomposite (MF + L) exhibits synergizing cytotoxic effects on the cells of MCF -7 line, that results in death of up to 40 % of cells.

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Lifetime positron spectroscopy of epoxy-unoxidized graphene composites

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An origin of structural-feature formation have been investigated in a DGEBA-epoxy resin-based composites filled with multilayered graphene nanoplatelets (MLGPs). MLGPs have basal surface size of about $5 \times 5 \mu\text{m}$, average thickness of about 50 nm, and number of graphene layers in a nanoplatelet was about 100. Structural rearrangement reveals itself in decreasing thermal stability with increasing graphene mass-concentration C and in anomalous behavior of the real part of dielectric permittivity at $C \approx 2$ wt.%. Nanoscale structural variations of epoxy molecular structure have been studied using the lifetime positron annihilation spectroscopy. The lifetimes τ_1 of quasi-free positrons, τ_2 and τ_3 of defect-captured positrons and positronium atoms (Pt), respectively, along with their annihilation intensities $I_{1,2,3}$ have been measured and presented in the Table with the evaluated average lifetime τ_{av} and radius of Pt-trapping defects R_{Ps} ,

Table. Annihilation parameters

C , %	I_1 , %	I_2 , %	I_3 , %	τ_1 , ps	τ_2 , ps	τ_3 , ps	τ_{av} , ps	R_{Ps} , Å
0	53.23	31.96	14.82	199.6	527.0	1670	522.1	2.522
1	52.86	31.82	15.32	199.4	503.0	1627	514.6	2.476
2	49.66	34.52	15.82	190.7	473.5	1581	508.3	2.426
5	52.68	32.45	14.88	199.9	489.0	1597	501.6	2.443

It was established that a rearrangement in composite's polymer structure occurs in the mass-concentration range of $C \leq 5$ % and is accompanied with a smooth enhancement in the electron density and monotonous decreasing of the free volume. Also, a formation of nano-sized vacancies and related redistribution in electron density among polymer macromolecular chains increase spontaneously within the range of $1 < C \leq 2$ %. Such local structural rearrangement induced by multilayered graphene platelets leads to noticeable variations in physical parameters of the composite at $C \sim 2$ %.

Evaluation of cardioprotective action of nano-antioxidants based on graphene oxide and its nitrogen-containing derivatives

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The screening of the compounds that help to reduce the degree of oxidative-nitrosative stress and reperfusion damage to the myocardium remains an urgent task of experimental cardiology. The effect of nanosized graphene as a potentially new, highly effective antioxidant on myocardial resistance and oxygen consumption by isolated rat heart in *in situ* ischemia-reperfusion model was investigated. Graphene oxide and its nitrogen-containing derivative were dissolved in Krebs-Henselait solution and injected into the tail vein at a dose of 0.03 mg / kg 30 min before decapitation. It was found that the original sample of unmodified graphene oxide showed a strong cardioprotective effect, which was manifested as a more complete restoration of myocardial contractile function and prevention of inefficient oxygen utilization by the ischemized heart. Thus, at the 5th min of reperfusion, left ventricle pressure was restored to 77.7 % and at 40th min was 76.5 % (against 34.0 and 42.7 %, respectively, in the control group). The maximum rate of myocardial contraction at the 5th min of reperfusion was 87.0 %, and at the 40th min - 93.0 % (against 32.8 and 42.6 %, respectively, in the control). The minimum value of dP/dt was 87 and 93 % versus 27.0 and 41.8 % in control. At the 5th min of reperfusion, coronary flow was 132.0 %, and at the 40th min - 89.1 %, which was greater than in control group (93.8 and 63.0 %, respectively). In the control group, at the 5th min of reperfusion, the oxygen cost of myocardial work increased in 5 times and decreased to 200 % from the base line at the 40th min of reperfusion, while in graphene pretreated group at the 5th min of reperfusion, it increased only by 10 % of baseline, indicating a powerful antioxidant effect of the selected dose of graphene. Intravenous administration of nitrogen-containing graphene had a similar protective effect on postischemic disturbances of the heart function and oxygen utilization.

Thus, our data reveal strong anti-ischemic properties of graphene oxide and its nitrogen-containing derivative that opens the prospects of their use to prevent myocardial dysfunction in ischemia-reperfusion.

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Heterogeneous recombination of H-atoms on a wide-gap catalyst with metal nanoclusters

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Heterogeneous catalytic reactions consist of separate chemical and physical elementary stages. Their effective rate depends on many factors, in particular, on the relaxation rate of the excited reaction products. Along with the one-quantum mechanisms of vibration-phonon relaxation of vibrationally excited molecules on the surface, a high-energy capture by the catalyst in one elementary act of a significant part of the energy released in the acts of chemical transformations takes place. This leads to electronic excitation of the surface. The generation of electronically excited states in catalysts is manifested in the phenomena of heterogeneous chemiluminescence, chemoemission, *etc.* On wide-gap catalysts, the electronic channel of the reaction energy accommodation is weakly manifested, while on metals it is the main one.

This work considers the reaction of recombination of H-atoms on a wide-gap catalyst. It was found that H_2^v migrate over the surface for a path length l of several tens of nanometers. Large values of l indicate the limiting role of relaxation of vibrational energy, as well as a low rate of accommodation along the phonon channel. If metal nanoclusters are placed on the catalyst surface at a distance equal to l , then relaxation of hot molecules via the electronic channel will occur on them. This will lead to an increase in the reaction rate if the processes of relaxation of the reaction energy limited the reaction rate.

The mathematical description of the general catalytic process is rather difficult due to the mutual influence of physical and chemical processes and was carried out using asynchronous cellular automata (CA). A CA-model is built, which describes the kinetics of the process in real physical time and uses physical cross sections and interaction constants. This made it possible to simulate not only the reaction itself, but also the nanocatalyst.

Thus, the implementation of the activation of the reaction on a substrate, and the processes of relaxation of excited states on nanoscale metal structures, is the basis for the development of catalysts with distributed functions of the processes of accommodation and relaxation. This approach gives a new insight on how to describe a whole class of studies in nonequilibrium catalysis and adsorption, where the processes of electronic accommodation have not been considered until now.

Catalytic activity of halloysite nanotubes decorated with nanoceria

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Nanoceria with unique structure and high catalytic activity has been used for a diverse range of applications in solid oxide fuel cells, sensors, catalysis, and nanomedicine. The ability to switch the oxidation state between ions Ce^{3+} and Ce^{4+} on the nanoparticle surface leads to the formation of oxygen vacancy that makes nanoceria highly efficient for enzyme-like catalytic activity. To prevent a reduction in the number of these oxygen vacancies due to the agglomeration of nanoparticles, halloysite nanotubes (HNT) can be modified by nanoceria, as they are biocompatible, environmentally friendly, and cheap. This work was aimed to obtain HNT/cerium oxide nanocomposites with different modifier content, to analyze their physicochemical properties, to experimentally determine the catalytic enzyme mimetic activity of the synthesized materials in a model reaction of hydrogen peroxide decomposition in comparison with the activity of nanoceria, pristine HNT, and catalase enzyme, to determinate the effective activation energy of the reaction of hydrogen peroxide decomposition by synthesized nanocomposites, HNT, and nanoceria.

Nanocomposites HNT/cerium oxide were synthesized by deposition of cerium nitrate in aqueous solutions at room temperature. The amount of nanoceria deposited in nanomaterials is 0.99–19.15 %, and their size varies from 2.6 to 17.5 nm. Electron diffraction studies of modifying particles in the samples indicate the cubic structure of cerium dioxide. The $\text{Ce}^{4+}/\text{Ce}^{3+}$ ratio in nanocomposites, estimated from UV-spectra of diffuse reflectance, increases from 0.25 to 2.55 with increasing of ceria content in nanocomposites. The catalytic activity of synthesized materials was studied in the reaction of H_2O_2 decomposition at different concentrations (1-10 %) at room temperature and within pH 8-11. The pH dependence of the nanocomposite's activity was shown to be extreme with maxima at pH 10.0. The highest catalytic activity is demonstrated by a sample that contains 3.19 % CeO_2 . Probably, decreasing the amount of decorator leads to a decrease in the degree of crystallinity, and an increase in the content of CeO_2 – to aggregation of particles, reducing the specific surface area, as a result – the number of surface defects (the measure of which is the ratio $(\text{Ce}^{4+}/\text{Ce}^{3+})$) decreases. Despite expectations, the activation energy of the hydrogen peroxide decomposition does not decrease with increasing sample surface defects but decreases with the increasing modifier content in the HNT/ CeO_2 nanocomposite.

Quantum-chemically computed integral characteristics of complex nanomaterials

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Development of additional theoretical tools to analyze electronic structure of complex nanomaterials depending on features of their spatial and chemical organization is of interest both from practical and theoretical points of view. Therefore, in this work, the development of an approach based on computations of the charge distribution functions (CDF, Fig.) in parallel to calculations of the distribution functions of the chemical shifts (SDF) of protons is carried out to be applied to a set of complex nanomaterials. Binary nanooxides (alumina/silica, titania/silica), 3d-metal-doped anatase, functionalized activated carbon, carbon nanotube, fullerene C₆₀, graphene oxide, and N-doped graphene are considered here as representatives of different classes of complex nanomaterials. The analyses of the CDF and SDF for certain kinds of atoms in complex systems provide a deeper insight into electronic structure features depending on composition of the materials, guest phase-doped host phase at various amounts of dopants, structure of O- and OH-containing surface sites (Fig.), amounts and organization of adsorbed water molecules, formation of charged surface functionalities and solvated ions, *etc.* The CDF of metal and hydrogen atoms (electron-donors) are more sensitive to the mentioned factors than the CDF of O, N, and C atoms (electron acceptors) in various systems. As a whole, the use of the CDF and SDF in parallel expands the tool possibility in detailed analysis of the structural and interfacial effects in dried and hydrated complex nanomaterials.

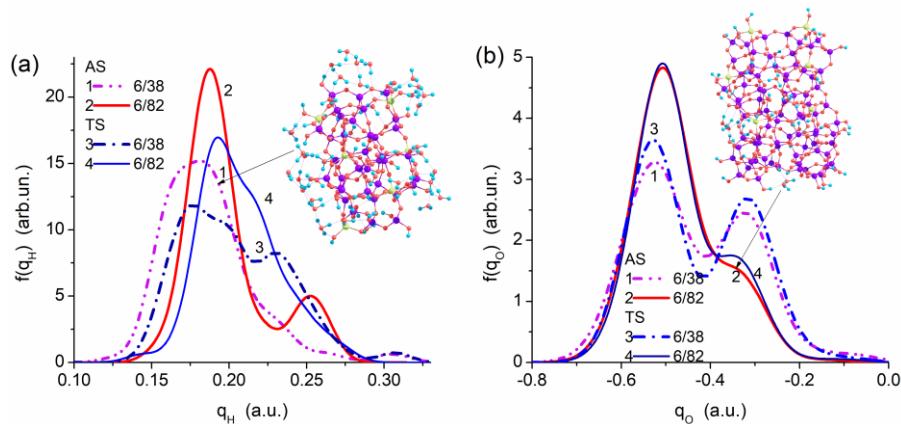


Fig. Atomic charge distribution functions in the clusters of Al₂O₃/SiO₂ and TiO₂/SiO₂ with 44 units (with 30OH and 24OH, respectively, and bound 42H₂O) and 88 units (46OH and 40OH, respectively, and bound 10H₂O) with six units of Al₂O₃ or TiO₂ for (a) H and (b) O atoms (DFT method with ωB97X-D/cc-pVDZ)

Biodegradable nanoporous polyhydroxybutyrate created by using nuclear technologies

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Today's global scientific trends in the field of membrane technologies are aimed at replacing synthetic porous materials with natural ones. Therefore, the development and research of porous materials based on polymers of microbial origin is extremely relevant and promising.

In the present work porous structure in polyhydroxybutyrate (PHB) films was generated by exposing PHB thin films (thickness was ~ 30 µm) to alpha (α) particles followed by simple chemical etching of the irradiated PHB films by using CHCl₃/MEK=70/30 (wt.%) solution for 2 hrs. depending on duration of exposing. The track-etched nanoporous PHB films obtained had average pore diameters in the range from 35 to 65 nm. The typical view of nanoporous PHB films obtained is shown in Fig. Increasing exposing time resulted in broadening pore size distribution from 20-90 nm to 15-140 nm, and increasing total porosity from 0.50 to 0.74 cm³/g (DSC-based thermoporometry data).

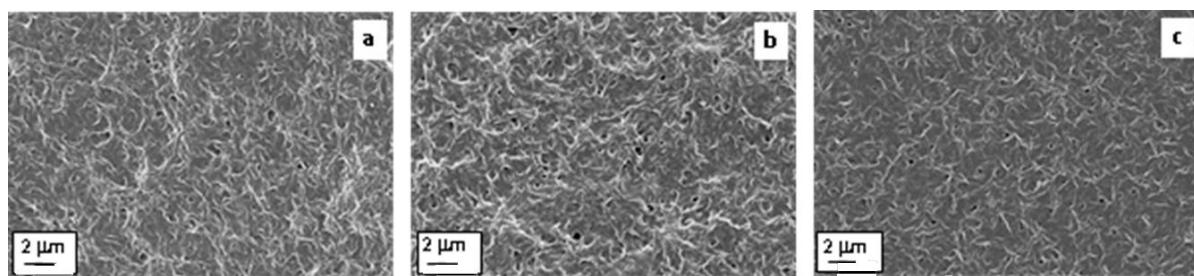


Fig. SEM micrographs of surfaces of the etched nanoporous PHB films exposed for 330 sec (a), 450 sec (b), and 690 sec (c)

Acknowledgements

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The effect of alkaline, acid and steam-explosion pretreatment of walnut shells and apricot seed shells on lignin yield

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Nowadays, it is necessary to develop new resources of raw materials for obtaining valuable products because of the depletion of natural resources of oil. A growing interest in the development of newest methods for the obtaining of different chemicals and fuels from renewable sources is observed worldwide. Of especial concern is the biochemical conversion of lignocelluloses. The aim of the research work is the investigation of the effect of different pretreatments of walnut shells (WS) and apricot seed shells (ASS) on the enzymatic hydrolysis and lignin yield.

The pretreatment with 1 % H₂SO₄ and 15 % NaOH (w/v) was carried out in reactor at 180 °C during 20 min (40 min was needed to reach the target temperature). The steam-explosion was performed in a custom-built batch pilot unit charged with 500 g of sample and heated with saturated steam to reach 180 °C, the process time was 10 min. The solids after pretreatments were used as substrates for enzymatic hydrolysis. Prepared materials were hydrolysed with industrial cellulase Cellic CTec2 enzyme cocktail.

The maximum lignin content of 82 % was achieved during enzymatic hydrolysis of solid after acid pretreatment of apricot seed shells due to the greater content of lignin in solid before the process. Despite the maximum efficiency of glucose conversion, the final sample of solid after alkaline pretreatment of apricot seed shells contains a minimum amount of lignin, among other samples based on this raw material. In general, the resulting solids together with lignin contain significant portion of substances of polysaccharide nature.

Acknowledgements

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Calculation of optical spectra of structures with silicon nanowires and silver nanoparticles

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When silver nanoparticles are added to the structure with silicon nanowires (Fig. 1), a decrease in the transmission coefficient is observed. The appearance of a new minimum can serve as confirmation of the appearance of surface plasmon resonance in the structure at a wavelength of 870 nm. This also increases the absorption coefficient of the studied structure (Fig. 2).

To exclude the peaks introduced into the absorption spectrum due to the Fabry-Perot effect, the absorption spectrum of only the silver nanoparticle layer was calculated to find out their contribution to the absorption spectrum of the structure itself. As can be seen (Fig. 2), it is the peak at a wavelength of 870 nm that contributes to the increase in the absorption coefficient of the whole structure.

It can be argued that the introduction of silver nanoparticles into the structure with silicon nanowires, promotes the appearance of localized surface plasmon resonance at wavelength of 870 nm, which significantly increases the absorption coefficient of the entire structure at this wavelength. And also increases the absorption coefficient in the range of 800-1000 nm (Fig. 2).

Such structures can be used in solar cells, significantly expanding their light trapping in wide range of wavelengths.

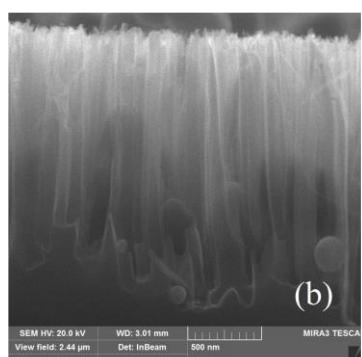


Fig. 1. SEM images of Si NWs with Ag nanoparticles

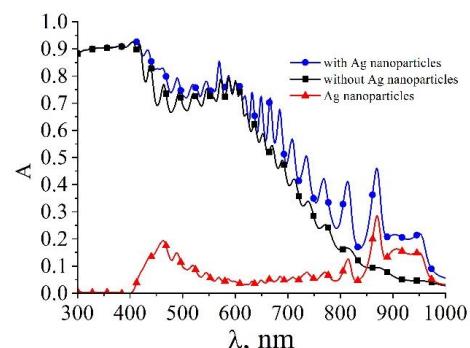


Fig. 2. Absorption spectra of silicon structures with silicon nanowires and silver nanoparticles

Clustering of printed electronic circuits elements: A formal percolation approach

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Electrically conductive polymer compositions are widely used in the creation of printed electronic circuits. Electrically conductive adhesives, pastes, enamels, plastics, elastomers and others are successfully used for this [1].

As is known, any electrical circuit can always be reduced to the form of a mixed (parallel-sequential) connection of elements. It is important that the topological organization of such schemes most closely resembles a hybrid of lattices with square and triangular cells, on which two-dimensional percolation problems can be solved.

Percolation theory [2, 3] investigates the structure and properties of connected regions or groups of similar (homogeneous) elements. Just such groups (having properties of physical clusters) are also formed by elements of percolation-modified electronic circuits too.

Research have shown that the cluster system of reformatted electronic circuits on a hybrid lattice is clearly visible. Percolation analysis of such a system allows, in addition to geometric parameters, investigating its electrical conductivity [4], obtaining a critical power index, and calculating the fractal and chemical dimensions of the skeleton of an infinite cluster and its lacunarity.

The purpose of further research of formatted electronic circuits is to identify non-trivial percolation-type dependencies between the structure and properties of electronic device circuits.

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Stimulating film coatings for seeds based on mixtures of silica and biopolymers

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In recent years, there has been a tendency to minimize the amount of mineral nutrients introduced into the soil. This can be done by spot application of fertilizers separately for each plant during its growth and vegetation, or by pre-sowing treatment of seeds with composite materials with a micro amount of fertilizers. The simplest is the method of pre-sowing seed treatment, it does not require special expensive equipment and qualified specialists.

The aim of this work was to develop a new generation of paste-like composite stimulating materials based on mixtures of hydrophilic A-300 and hydrophobic AM-1-300 silicas with trace amounts of mineral fertilizers and a biopolymer component for pre-sowing seed treatment.

Composite materials for pre-sowing seed treatment were prepared by thoroughly grinding a mineral matrix (a mixture of hydrophilic and hydrophobic silicas in a ratio of 1:1 and 2:1) with a micro-amount of mineral fertilizers and a solution of a biopolymer (gelatin). Such composite systems were applied directly to the surface of the seed, wheat grains of the "Natalka" variety, before being exposed in sand and on filter paper, according to DSTU 4138-2002. During the study period, the following parameters were measured: seed germination energy, germination and morphological characteristics of wheat germs, which consisted in measuring the length of the root and stem.

It was found that wheat kernels treated with a 2:1 paste with stimulating antifungal additives have a maximum sprout length. Sprouts of caryopses treated with 1:1 pastes have average values. The smallest lengths are observed for sprouts whose caryopses were treated with composites 2:1 (without antifungal components).

The most uniform seedlings are observed for wheat germ treated with a paste based on a 1:1 mixture with the components of biofungicidal preparations.

The thermodynamic interactions in the POSS-containing nanocomposites based on PU/PHPMA semi-IPNs

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The impact of different amount of the 1,2-propanediolisobutyl-POSS (POSS) on the thermodynamic state of the nanocomposites based on semi-interpenetrating polymer networks (semi-IPNs) of the crosslinked polyurethane (PU) and linear poly(hydroxypropyl methacrylate) (PHPMA) have been investigated.



Fig. The isotherms of dichloromethane vapour sorption (*a*) and free energy of mixing Δg^m (*b*) of samples with dichloromethane; x/m is the amount of dichloromethane relative to the dry sample; p/p_0 is the relative pressure of dichloromethane; ω_2 is weight fraction of solvent in the sample

With the aim to estimate the thermodynamic state of the semi-IPN-15 nanocomposites the dichloromethane vapour sorption by the samples was studied using a vacuum installation and a McBain balance (Fig. *a*). The isotherm of semi-IPN-15 is between the two extremes for the individual polymers. With increasing amount of POSS in the samples the values of vapour sorption is less in compare with native matrix, this means the formation of more dense structure of nanocomposites with high POSS content.

The thermodynamic parameters are calculated from the experimental data of isotherms of sorption. In Fig. *b* the changes of the free energy of mixing Δg^m of solvent with polymers are presented. The free energy of PU and PHPMA mixing was calculated based on data of Fig. *b*, and was shown it is positive. This means the thermodynamic incompatibility of semi-IPN's components. The introduction of 1-3 wt.% of POSS lead to futher phase separation in semi-IPNs. This is due to concentration of POSS particles in the PU's nanodomain. The increasing of POSS content to 5-10 wt.% lead to compatibilization in semi-IPNs - the free energy of component's mixing became negative. These due to concentration of POSS nanoparticles not only in the PU's nanodomain but also in the interphase region of semi-IPN.

Modification of hemostatic powders based on alginate and dispersed silica with Ag and Ag/Cu nanoparticles

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The current level of military conflicts in the world and the need to save lives require the development of new highly effective materials, including hemostatic dressings, which are important for wound healing and stopping bleeding. The problem of giving such materials antibacterial properties is also actual. Antibiotic resistance to antimicrobial drugs has a negative effect on the treatment of patients, so the urgent problem is the search for biocidal and hemostatic drugs). Alginate-based dressings show high hydrophilicity, the high bactericidal ability of nanosized silver is well known, as well as the high sorption capacity of highly dispersed silica (HDS) (like three in one). The combination of these three parameters can create a unique material with new healing properties. We created a composite material by combining 3 components with useful properties based on sodium alginate, HDS and nanoparticles of silver and copper for use in hemostatic/bactericide dressings. Ag nanoparticles and Ag/Cu composite were introduced into an aqueous suspension of HDS with sodium alginate, then dried using a rotary evaporator under heating. Similarly, a series of samples was obtained where Ag⁺ and Ag⁺/Cu²⁺ ions were introduced into the suspension. Due to the presence of glycosidic groups, sodium alginate exhibits reducing and protective properties for metal nanoparticles, while nanodispersed silica acts as a spacer, limiting the growth of nanoparticles by adjusting their size. The obtained materials were characterized by X-ray, optical and infrared spectroscopy methods. The composites showed high hemostatic and bactericidal properties in laboratory tests on rats.

The quantity and quality of Ag nanoparticles and Ag/Cu composite do not reduce the hemostatic properties of combined powders, but give them bactericidal properties

On the properties of highly-doped ZnO:Al,N films grown at oxygen-poor and oxygen-rich conditions

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Recent years ZnO due to its inexpensive, non-toxicity growth technologies still has been intensively studied as a perspective material for the development of optoelectronic devices because of its wide-band gap of 3.3 eV and large exciton binding energy (60 meV) at room temperature [1]. The study of the effect of oxygen-poor and oxygen-rich conditions at the deposition of highly-doped ZnO:Al,N films on the defects formation is an attractive for the understanding and obtaining *p*-type conductivity in ZnO as well as for an improvement of performance of ZnO-based ultraviolet heterojunctions.

Hence, highly-doped ZnO:Al,N films were grown under oxygen-poor and oxygen-rich conditions on Si substrates by magnetron sputtering using a layer-by-layer growth technique [2]. X-ray diffraction, scanning electron microscopy, energy dispersive X-ray analysis, X-ray photoelectron spectroscopy, X-ray emission spectroscopy, Raman scattering, photoluminescence [3] and Secondary ion mass spectrometry were used for the samples characterization. The effect of high aluminum and nitrogen doping on the structure, optical and electronic properties of ZnO:Al,N films deposited under oxygen-poor and oxygen-rich conditions was studied. The results will be discussed.

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Formation of the physicochemical properties of nanodispersed diamond powders with a chemically uniform surface

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Nanodispersed diamond powders are widely used in modern technological processes in the production of polishing suspensions, pastes, adsorbents and other materials. The use of nanodiamond powders with specified physicochemical properties is one of the main requirements for the materials being created.

Physicochemical properties of nanodispersed diamond powders of static and detonation synthesis have been studied in detail at the V. Bakul Institute for Superhard Materials National Academy of Sciences of Ukraine in recent years.

It has been established that the physicochemical properties of nanodispersed diamond powders are associated with the inhomogeneity of the chemical composition of the surface. The heterogeneity of the chemical composition of the surface of nanodiamond powders is closely related to the nature, quantitative composition of bulk impurities, as well as the nature and amount of compounds and functional groups on the surface. The bulk impurities are impurities of metals and metalloids remaining in nanodiamond powders after their manufacture. Impurities that are contained on the surface of a diamond are adsorbed compounds and functional groups, for example, hydroxyl, carbonyl, carboxyl and other groups.

It is proposed to evaluate the chemical heterogeneity of the surface of nanodiamond powders by the value of the criterion K . The criterion characterizes the fraction of the specific surface of nanodiamond powder, which is occupied by conductive centers. Criterion K is the ratio of the area of effective conductive centers of the original and reconstructed surfaces of nanodiamond powders. It has been established that the lower the K value, the better the nanodiamond powders are purified, the less incombustible residue in them and the lower the content of functional groups present on the surface. For example, a special chemical treatment of the initial powders of nanodiamonds of the ASM grade with a grain size of 0.1 / 0 leads to a decrease in the incombustible residue from 1.61 to 0.63 %. Criterion K decreases from 13.7 to 4.6.

Thus, special methods of chemical, thermochemical and electrochemical surface treatment of nanodispersed diamond powders make it possible to obtain powders with a high degree of chemical surface homogeneity.

Therapeutic and prophylactic drug against anemia of animals

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Method preparation of medical and preventive oral preparation against animal anemia was elaborated, which foresees:

- The use of freshly-prepared iron carbonate paste synthesized via interaction of $\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$ and NaHCO_3 (as a source iron(II) - main active component);
- Interaction of iron carbonate and cobalt chloride with complex formation with monosaccharide *D*-fructose having hemo-stimulating properties;
- concentrating of complex solutions up to syrup consistency, its extraction from reaction area in the free state using alcohol-ether mixture, its treatment with acetone, ether, and drying in vacuum conditions;
- infliction of complex mixtures containing certain quantities of Fe(II) fructose and Co(II) fructose with aqueous Askan-clay (through ultrasonic material dispersion); preparation of water suspension, its drying, grinding, manufacturing of solid form of preparation for oral administration.

The preparation manufactured by mentioned method contains (in mass %): ligand *D*-fructose 24.2-29.0; iron(II)- 7.5-9.0; cobalt(II)- 0.0007; natural Askan-clay 68.3-62.0.

The offered method provides getting of highly digestible, antistress, preparation with high bio-accessibility (bio-digestibility) and low toxicity intended for oral administration, as well as a functional targeted product with maximum content of Fe(II).

Experiment result was expressed in getting rid of complications (iron deficiency anemia, diarrhea-dyspepsia) caused by stress factors related to termination of breast feeding of store pigs and food change, as well as in their normal growth and development, normal blood chemistry values and live weight gain.

Chitosan-based QCM sensing system for vapor analysis

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Quartz crystal microbalance (QCM) sensors can be used to detect indoor pollutant vapors quickly and easily, as they can measure the weight change caused by the analyte sorption on the sensitive material down to nanograms, resulting in a frequency shift. Various materials (polymers, metal oxides, *etc.*) are used to modify the sensors surface. Chitosan with a large number of free amino and hydroxyl groups, mechanical strength and film-forming properties, is a good candidate for this. In our work, chitosan was used as a sensitive material for detecting vapors of alcohols (methanol, ethanol, butanol, isopropanol) and acetone. The sensing mechanism can include absorption-desorption processes (hydrogen bonds of protonated amino groups or hydroxyl groups). We used the QCM setup based on the QCM100 microbalance unit (Stanford Research Systems, USA) and original data acquisition system developed in the Institute of Applied Physics. Chitosan (300 kDa) was applied to the cysteine layer; glutaraldehyde was used as a cross-linking agent, as described in [1].

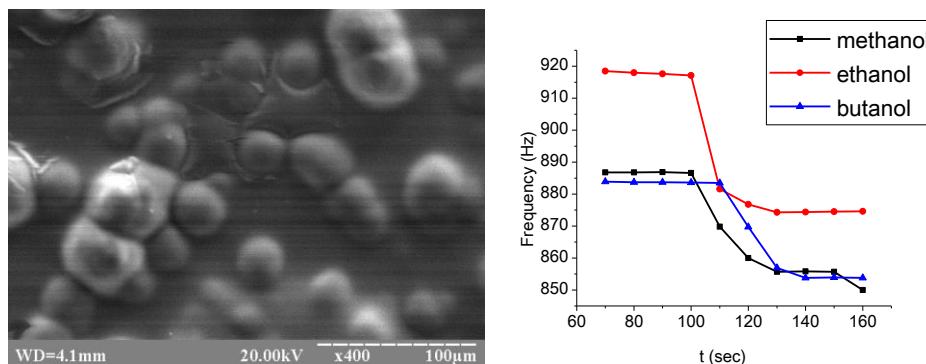


Fig. The surface of the sensor (left) and the response profiles for different alcohol vapors (right)

The sensor's response (frequency shift) depends on the nature of alcohol vapor (Fig.). Among tested alcohols, ethanol gives the maximal shift (52 Hz), while isopropanol and acetone do not cause any response at all. The sensor is also very sensitive to water vapors, so the relative humidity should be monitored.

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TPDMS study of casein-calcium carbonate particles

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Disperse imitators of fat globules are in demand in the production of products with a reduced fat content. In our study, we used calcium carbonate (5 microns, 99.5 %, Alfa Aesar) as the core of the particles, casein isolated from milk (without additional skimming) and Casein acc. to Hammarsten. Calcium is an essential mineral for human nutrition. Calcium carbonate, the most stable and widespread form of calcium, has disadvantages (low solubility and sensory defects) that prevent it from being incorporated into liquid foods. Correctly engineered ultradisperse particles can solve many of the problems of calcium incorporation in foods. It is known that phosphoproteins have a specific effect on the crystallization of calcium carbonate. In our study, the interaction between calcium carbonate and casein was investigated by the TPDMS method.

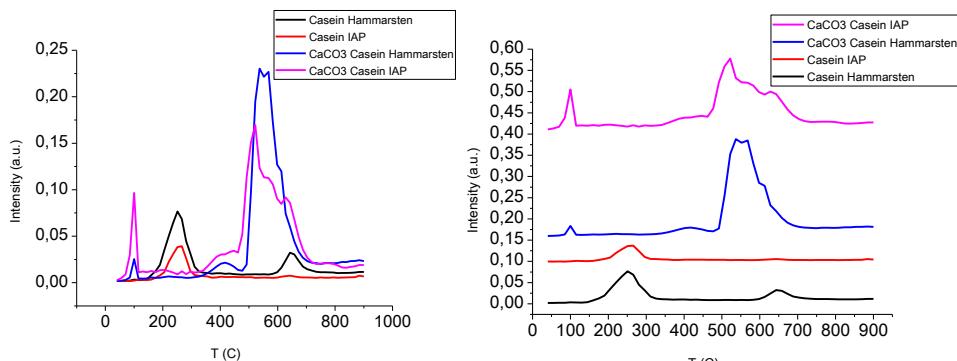


Fig. Temperature dependant CO₂ evacuation profiles of different caseins and calcium carbonate-casein particles

The SEM images of the dried casein-calcium carbonate particles show that they comprise two kinds of particles: small particles 2-5 μm in size and bigger particles with sharp edges 10-30 μm (much less numerous). Thermal behavior of caseins and calcium carbonate casein particles strongly depends on the components sources and the preparation protocols (Fig.).

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Chitosan based nanostructured materials for medicine

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Chitosan-based materials have attracted considerable attention in the field of biomedicine due to their unique biodegradable, biocompatible, non-toxic and antimicrobial nature. Chitosan is an ideal biomaterial for antimicrobial dressings, which can either be manufactured separately in their original form, or be modified to include antibiotics, metal antimicrobial particles, natural compounds and extracts to enhance antimicrobial action. In the Institute of Applied Physics of the National Academy of Sciences of Ukraine, for a long time, the synthesis and study of materials based on chitosan for medical purposes has been carried out: films, coatings, sponges, composite materials with inorganic components (magnetite, hydroxyapatite), sorbents, etc. The use of lyophilization, treatment of materials with the femtosecond laser, proton and electron beams makes it possible to create fine structures on the surface of the materials, giving them new properties (see Fig.).

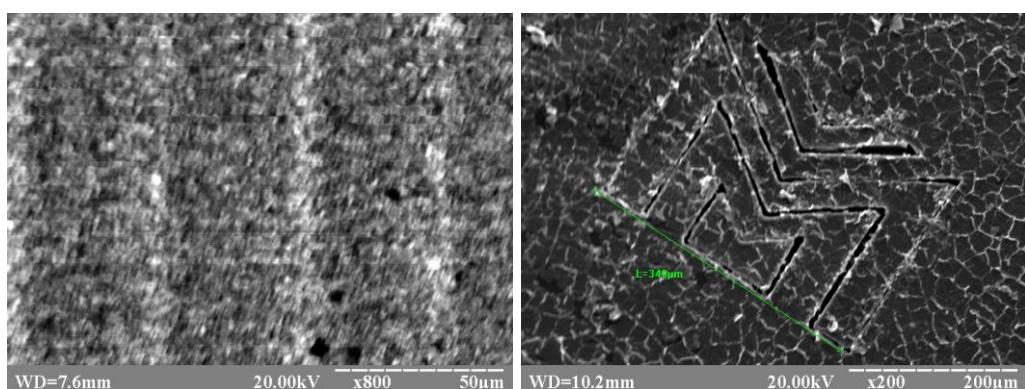


Fig. Chitosan film with Ti layer deposited by magnetron sputtering: periodic structures on its surface created with the femtosecond laser treatment (left) and the structures made by proton beam writing (right)

The effect of an oxide layer on surface plasmons in metal 1D structures

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The current level of technology development provides unprecedented opportunities in the manufacture of various nanoscale elements, which led to the emergence and development of nanoplasmonics. This is due to the fact that the enhancement of the field in the vicinity of metal nanoparticles causes a number of specific phenomena and significantly increases the detection threshold of optical signals from various objects located near the surface of the nanoparticles [1]. One of these specific phenomena is surface plasmon resonance (SPR), the spectral position of which strongly depends on both environmental parameters and the geometric shape and composition of nanoparticles [2]. In this regard, the use of various sensors of metal 1D structures as sensitive elements is promising. Of particular interest is the study of the effect of the oxide layer on the SPR characteristics in metal wires.

Using the condition of plasmon resonance for the case of a metal-oxide nanowire and the Drude formula for the dielectric function of a metal, the equation for determining the dimensional dependence of the frequency of surface plasmons can be written in the form

$$\omega_{sp} = \sqrt{\frac{\omega_p^2}{T^\infty + T_{ox} \frac{(1+\beta_c)T_m + (1-\beta_c)T_{ox}}{(1+\beta_c)T_{ox} + (1-\beta_c)T_m}} - \gamma_{eff}^2}, \quad (1)$$

where ω_p – plasma frequency; T^∞ – component describing the contribution of the ionic core of the metal; γ_{eff} – effective relaxation rate, equal

$$\gamma_{eff} = \gamma_{bulk} + \gamma_s = \gamma_{bulk} + \frac{9\pi(3\pi)^{\frac{1}{3}} v_F}{64 a}. \quad (2)$$

Here γ_{bulk} – the rate of relaxation of electrons in a 3D metal; v_F – electron Fermi speed; a – radius of the metal core.

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Preparation of perovskite-type solid-solutions applying sol-gel synthetic approach

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Materials with perovskite-type structure can be applied in many different fields, including superconductors, photocatalysts, thermoelectrics, chemical sensors [1] or multiferroics [2]. In recent years perovskites with multiferroic features have attracted more and more attention due to captivating physical properties and possible implementation in technology in both single-phase, or solid solutions forms.

While solid-state synthesis is a well-known technique for preparation of various inorganic oxide materials, it still has some difficulties, like formation of impurity phases, which are hard or impossible to separate, achievement of homogenous dopants distribution or usage of high temperature and pressure. All of these problems can be solved applying environmentally-friendly, low-cost aqueous sol-gel technique, which is considered as a soft chemistry route.

In this work, two different solid solutions series $Y_xGd_{1-x}Mn_{0.97}Fe_{0.03}O_3$ and $Y_{1-x}Gd_xFeO_3$ were prepared via sol-gel synthetic approach. Different characterization techniques were employed in order to investigate structural, morphological and magnetic properties of these compounds.

Acknowledgements

This work was supported by a Research grant BUNACOMP (No. S-MIP-19-9) from the Research Council of Lithuania.

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Photocatalytic effect of ZnO nanostructures grown on Si, Ag/Si and Au/Si substrates by APMOCVD approach

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Semiconductor photocatalysis is one of the most important technologies used for the complete mineralization of a wide range of toxic chemicals. Being a wide-gap semiconductor material ZnO is considered as a good one for removal of hazardous materials such as dyes and organic compounds from waste water. ZnO nanostructures (NS) are promising photocatalysts because of their high redox potential, high quantum efficiency, a good physical and chemical stability. In addition, it is non-toxic and low-cost material, suitable for large-scale production.

The APMOCVD process was realized in quartz tube by decomposition of one gram of zinc acetylacetone precursor. ZnO NS growth was maintained at substrate temperature of 500 °C. The XRD, SEM, PL and Raman measurements were carried out for characterization of structure and optical properties of deposited NS. Photocatalysis of ZnO NS was studied by decomposition of metal-orange dye (MO) with initial concentration 10 mg/l upon UV Hg lamp irradiation with power of 200 W during 9 h. The results of dye degradation (% of dye decomposition) are presented in the Table. The best photocatalytic effect was observed for ZnO NS deposited on Si substrates coated by Ag thin film. Other obtained results like XRD, PL and Raman will be analyzed and discussed.

Table. Percent of dye decomposition for grown ZnO nanostructures

Time, hours	MO	Si substrate	ZnO/Si	ZnO/Au/Si	ZnO/Ag/Si
3	7.9	6.3	18.8	18.6	29.2
6	11.9	9.2	37.2	35.3	56.8
9	16.6	11.5	55.9	56.3	78.9

Acknowledgements

This work was partially supported by the research project of NAS of Ukraine “Development of innovative photocatalytic nanostructured materials based on ZnO and TiO₂” and was partially supported by the research projects of NAS of Ukraine “The development of photocatalytic nanocomposites for viruses inactivation in the air”.

Rheological properties of colloidal silicas prepared by ion exchange

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Suspensions based on nanosized silica particles are used for chemical-mechanical polishing of silicon wafers [1]. The preparation of highly concentrated stable slurries with low viscosity is cost effective. We offer ion exchange method of preparation of highly stable low viscosity colloidal silicas. The concentration increase of silica dioxide is achieved by adding nanosized particles ($d \approx 40$ nm) of fumed silica OX-50 (Evonik, Germany).

The rheological behavior of colloidal silicas has been investigated by rotational viscometry. Suspensions stabilized with sodium hydroxide or ethylenediamine are thixotropic with a rapid rate of restructuring (Fig.).

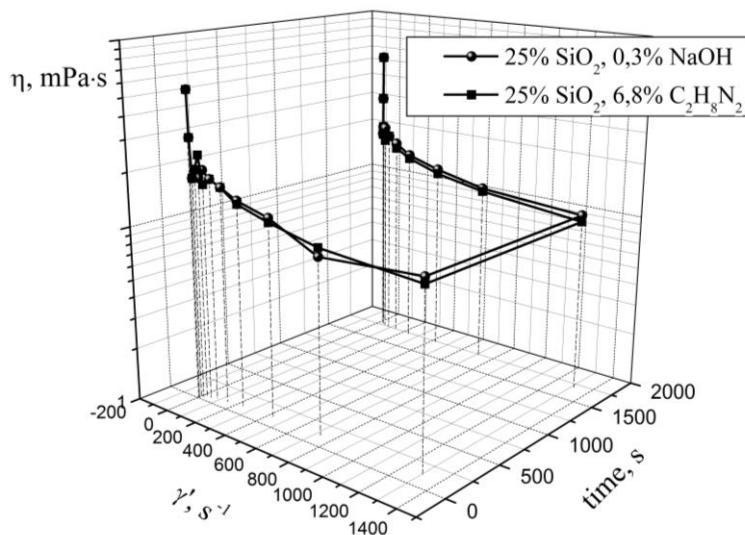


Fig. Viscosity as a function of shear rate and time for stabilized suspensions

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Peculiarities of gaseous toluene adsorption during photocatalytic air purification

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When studying the photocatalytic air purification from the harmful substance toluene by monitoring the change in its concentration, some authors do not take into account the probability of adhesion of this substance to the reactor walls, for examples [1,2]. However, our experiments have shown the fallacy of such an approach.

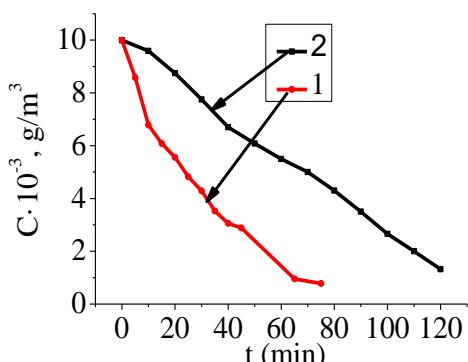


Fig. The dependence of the toluene concentration on the residence time in a glass reactor

The Figure shows the dependence of the toluene concentration on the residence time in a glass reactor with an inner surface covered with a 80 nm thick film of the photocatalyst ZnO:Ho (5 at.%) (curve 1) and, for comparison, with a 0.1 nm thick teflon layer (curve 2) in conditions of the absence of light irradiation and the ambient temperature and pressure.

As seen, the concentration of toluene in the reactor is continually decreasing, that is, its adsorption on the walls exceeds desorption

even at a long (over 1 hour) exposure time. Such an adsorption-caused decrease in the toluene concentration is observed not only on the ZnO:Ho (5 at.%) film, but also even on the layer of teflon, which is well known as a substance chemically inert to most reagents and having a weak adsorption capacity. The significant deposition of toluene, even on a surface with poor adhesion, is apparently associated with its high boiling point - 110.6 °C, due to which at room temperature of the reactor walls, toluene molecules intensively settle on the surface of any substance.

From the results presented, it becomes evident that when studying the photocatalytic activity by controlling the concentration of toluene, it is necessary to take into account the probability of its adhesion losses on the reactor walls.

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Magnetically sensitive multilayer nanostructured composites as adsorbents for isolation extracellular trehalose lipid surfactants

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Biosurfactants – environmentally safe compounds characterized by surface and biological activity, biodegradability and low toxicity. Among biosurfactants producers, actinobacteria *Rhodococcus erythropolis* Au-1, which synthesize trehalose lipid surfactants (TLs) at various locations, have practical potential [1]. However, the industrial production of TLs is limited, in particular, by the stages of isolation and purification of target products.

A new method for extracellular TLs isolation using nanostructured composite adsorbents has been developed. They have a magnetically sensitive core of cobalt ferrite, covered with a protective layer of porous SiO_2 , on the surface of which are clusters of transition metals oxides (CuO, CoO, MnO) [2]. Isolation of the target products includes: 1) sorption of TLs by composite adsorbents from cell-free culture fluid; 2) deposition under the action of a magnetic field; 3) extraction of TLs with a solvent. It has been shown that composite adsorbents make it possible to selectively isolate trehalose lipids. Thus, when using a composite with CuO was obtained 0.88 g/dm^3 extracellular TLs (Fig. 1). It was determined by thin layer chromatography (TLC) that they contained trehalose lipids without impurities of other substances (Fig. 2). The control method is less selective and more expensive due to the use of significant volumes of solvents. Extraction of TLs by Folch mixture (chloroform-methanol, 2:1 vol/vol) makes it possible to obtain 0.95 g/dm^3 TLs with a high content of non-polar lipids.

Therefore, a new effective method of extracellular TLs isolation has been proposed. Thus, the advantages of using composite adsorbents are the possibility of their repeated use after extraction of the target products and separation using an external magnetic field.

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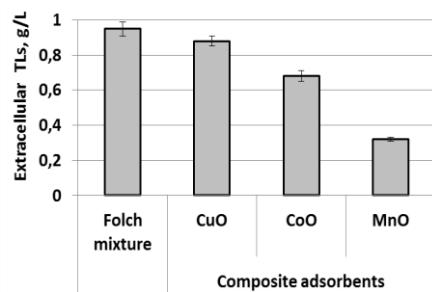


Fig. 1. The effectiveness of methods for isolating extracellular TLs of *R. erythropolis* Au-1 strain

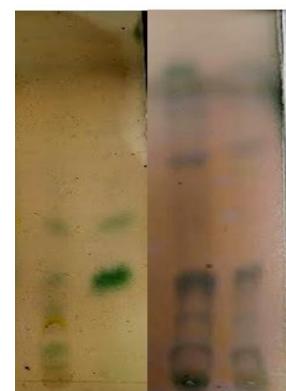


Fig. 2. TLC of extracellular TLs: extraction by Folch mixture (1) and sorption by composite adsorbents based on CuO (2), MnO (3), CoO (4)

Surface chemistry and adsorption properties of nanoporous carbon obtained by pyrolysis of carbides

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Carbon-derived carbon (CDC) is a new generation of carbon materials that are produced by thermal treatment of various types of carbides, such as titanium and silicon carbides, with chlorine. CDC is a carbon material, which structure varies from amorphous to crystalline. It is chemically stable and possess a tunable pore assembly. CDC surface properties can be adjusted by changing the preparation conditions and raw materials used for production.

In the present work the nanoporous carbon obtained by thermal treatment of titanium carbide powder was used. CDC was characterized by studying its morphology, chemical composition, surface area and the point of zero charge.

The surface area and pore size distribution in the CDC were evaluated by the BET method by using nitrogen sorption/desorption experiments. Surface functional groups on the CDC were determined by Fourier transform infrared spectroscopy. The morphology and chemical composition of the CDC were examined using an emission scanning electron microscope in combination with an energy-dispersion spectrometer. The point of zero charge of CDC particles was determined by measuring their zeta potential at different pH values of aqueous solutions from 2 to 12.

The efficiency of surfactants adsorption on the sorbent was also investigated. Anionic sodium hexadecyl sulfate (SHDS) of general formula $C_{16}H_{33}SO_4Na$ was used as a surfactant. Adsorption was investigated in the range of equilibrium concentrations not exceeding the critical micelle concentration of the surfactant. It was found that the adsorption capacity of CDC towards SHDS exceeds the capacity of other common carbon sorbents, such as graphite carbon black [1], and it is comparable to the capacity of activated carbon [2]. The adsorption mechanism, the effect of contact time and pH value on adsorption process have been considered and analyzed.

The performed adsorption studies with the anionic SHDS surfactant have revealed that CDC is a promising adsorbent for removal such type of pollutants from aqueous solutions.

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Alginate-magnetite nanocomposite hydrogels as drug delivery systems

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As a result of combining polysaccharide hydrogels with magnetic nanoparticles, hybrid hydrogels are formed. These new composite materials are of particular interest because they have the characteristics of both components, and most importantly the biocompatibility of polysaccharide matrices and the magnetic susceptibility of nanoparticles. As a result, such materials have a wider range of potential applications.

Magnetite nanoparticles were obtained by *in situ* syntheses in polysaccharide matrices of κ-carrageenan and sodium carboxymethylcellulose. Magnetically sensitive hydrogels based on sodium alginate and Fe₃O₄ nanoparticles were prepared by ionotropic gelation with calcium chloride as a crosslinking agent. Hydrogels with nanoparticles concentrations of 1, 2.5, and 5 % were obtained. Acetylsalicylic acid was chosen as a model drug.

In a constant magnetic field, the samples released acetylsalicylic acid more actively, as the porosity of the hydrogels is reduced due to the ordering of the magnetic particles, as a result of which the adsorbate molecules should be pushed out due to the pore narrowing. In a slightly alkaline environment, the alginate forms a soluble viscous gel, so the movement of magnetic particles inside it is facilitated, and the deformation and displacement of the adsorbed drug were more noticeable. Thus, the results of the experiment showed the acceleration of drug release under the influence of the applied constant magnetic field at pH 6.8.

At low pH, alginate collapses to form insoluble alginic acid. Thus, the resistance of the chains to deformation increases, which complicates the movement of particles in the polymeric grid. As a result, the magnetic particles impregnated in the alginate hydrogel reacted weakly to the action of the magnetic field when the film was immersed in a solution with a pH value of 1.6. The big difference between the degrees of swelling of hydrogels in such an environment when applying a constant magnetic field was observed due to the fact that, despite the complexity of the motion of particles, they still get their own magnetic moment as a result of magnetization and interact with each other forming a framework of nanoparticles, which maintains a constant volume of hydrogel and thus slows down the diffusion of acetylsalicylic acid molecules into solution.

Pickering emulsions stabilized with magnetite nanoparticles

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Pickering emulsions are dispersed systems stabilized by solid particles, which are fixed at the oil-water interface instead of conventional emulsifiers. Pickering emulsions gained their popularity due to the promising environmentally friendly and economical manufacturing of hybrid polymer particles and nanocomposites with supramolecular colloidal structures. They have a lot of advantages over emulsions stabilized by classical low molecular weight surfactants. Firstly, such emulsions are environmentally friendly and biocompatible, as they do not show toxic effects on living organisms. Therefore, the use of such emulsions corresponds to the principles of green chemistry. Secondly, they are resistant to coalescence and isothermal distillation. Moreover, the main advantage of Pickering emulsions is the ability to provide them with additional functions due to the properties of stabilizers - (bio)catalytic ones, sensitivity to various environmental factors, such as pH, temperature, ionic strength, magnetic field, etc.

Magnetite nanoparticles stabilized with sodium alginate with an average size of 20 nm were used as a stabilizer of the Pickering emulsions. For the preparation of emulsions, a solution of 2 % chitosan as an aqueous phase and vegetable oil as a non-aqueous phase were used. *p*-Aminobenzoic acid (PABA) was introduced into the chitosan phase as a model drug. Emulsions were obtained by the dispersion method at a stirring speed of 3000 rpm. The release of PABA was studied at different temperatures at pH 5.5, which corresponds to the pH of the skin.

Thus, the release of PABA from emulsions without the influence of a magnetic field occurs by the mechanism of delayed Fickian diffusion. Whereas the application of both constant and alternating magnetic fields significantly accelerates the release of drugs from emulsions and causes a change in the mechanism of PABA release to abnormal diffusion. The activation energy for the Pickering emulsion stabilized with magnetite nanoparticles was 76.8 kJ/mol, while for the unstabilized emulsion it was 29.5 kJ/mol.

Dynamic viscosity of polyvinyl chloride containing nanodispersed metal powders

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In the glassy state and the transition zone from the glassy state to the highly elastic molecular-kinetic nature and the dependence of the value of dynamic viscosity, energy dissipation on the content (φ) of nanodispersed copper in composites obtained on the basis of polyvinyl chloride (PVC), which undergoes longitudinal, shear and volumetric deformation by frequency $\omega = 0.4 \cdot 10^6 \text{ c}^{-1}$.

Using the Alfrey-Maxwell model, an analytical relationship was established between elastic, viscoelastic deformation and dynamic viscosity of PVC filled with nanodispersed copper powder in an amount of $0 \leq \varphi \leq 3,0$ vol.%. Under the action of active centers of the filler surface, nonlinear changes in the magnitude of the shear modulus, volumetric compression (tension), dynamic viscosity, and relaxation times of processes associated with the elastic and viscoelastic components of deformation of PVC systems are observed. The relative change in the value of these characteristics is determined based on the dissipative processes of energy exchange, using the relationship - deformation-frequency-temperature. The maximum effect of the influence of nanodispersed copper on the viscoelastic properties of PVC systems is observed in the range (0.05 ÷ 1.00) vol.% filler. The change in the linear dimensions of the structure formation, the factor of their anharmonicity is due to the energy component of the donor-acceptor interaction at the PVC-Cu phase interface. The study of the viscoelastic properties of a body in the megahertz frequency range and temperature range of $298 \text{ K} \leq T \leq 353 \text{ K}$ makes it possible to predict the conditions for obtaining and operating the material by the value of the dynamic viscosity of the body without destruction of the material under the simultaneous action of temperature and mechanical dynamic fields as dampers, acoustic delay lines, matching devices.

The effect of germanium citrate on the state of the pro- and antioxidant system of the mice liver in LPS-induced endotoxemia

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The development and application of protective and therapeutic agents for endotoxin-mediated inflammatory processes is an urgent problem. At present, organic compounds of germanium (Ge), which have a wide spectrum of biological action and certain protective properties, are being actively studied [1, 2]. In our work, to study the state of the pro- and antioxidant system of the mice liver under the conditions of lipopolysaccharide (LPS) induced endotoxemia, we used Ge citrate obtained via electropulse nanotechnology [3], which is characterized by environmental safety, high purity and bioavailability.

It was found that the introduction of LPS caused an increase in the content of TBA-reactive products (TBA-RP) in the liver tissue, which indicates an increase in lipid peroxidation (LPO). The amount of reduced glutathione (RGL) and the activity of ceruloplasmin (CP) in the blood serum significantly decreased under the conditions of LPS action. The use of Ge citrate in mice with endotoxemia led to a decrease in the amount of TBA-RP in the liver tissue ($p<0.05$ compared to LPS) and significantly increased the content of RGL ($p<0.05$) and CB ($p<0.05$). Obtained data indicate that Ge citrate has antioxidant properties under the conditions of endotoxemia.

Thus, the use of Ge citrate contributed to the weakening of oxidative stress in the liver of mice and improved the state of the antioxidant defense of the body, that is, it had a pronounced protective effect under the conditions of experimental endotoxemia.

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Immobilization of calcium pantothenate in water-oil emulsion by the membrane emulsification technique

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Water in oil emulsions is widely used in the food, pharmaceutical, and cosmetic industries. Membrane emulsification technique is a unique technique that is especially useful in preparing uniform-sized particles [1]. The size of the particles depends on the pores of membranes and membrane materials

In this work, the water-oil microemulsions based on chitosan was obtained by the membrane emulsification technique. Polyethylene terephthalate track-etched membranes (PET) with pore size of 0.1 μm were used for emulsion preparation. The influence of the main parameter on the drop size of microemulsions and their stability were studied. Calcium pantothenate was immobilized in the disperse phase of the microemulsion. The influence of pH and temperature on profile release of calcium pantothenate were studied (Fig.)

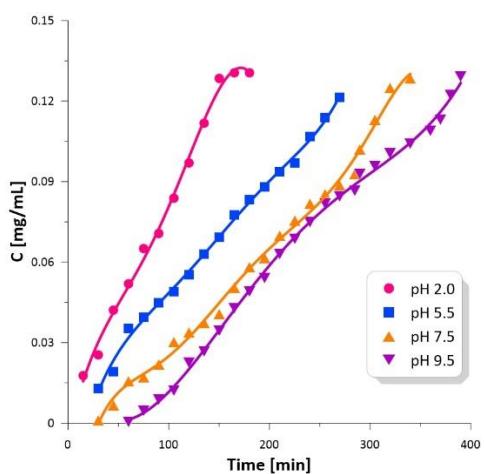


Fig. Kinetics of release of immobilized calcium pantothenate from chitosan microemulsions depending on pH: 2.0; 5.5; 7.5; 9.5 at temperature 37 °C

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Cisplatin adsorption on the surface of magnetosensitive nanocomposite $\text{Fe}_3\text{O}_4/\text{Al}_2\text{O}_3/\text{C}$

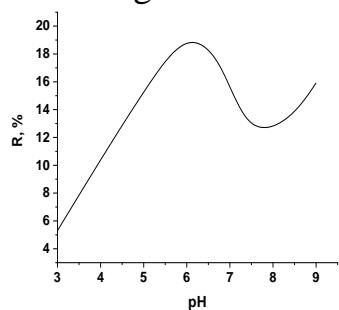
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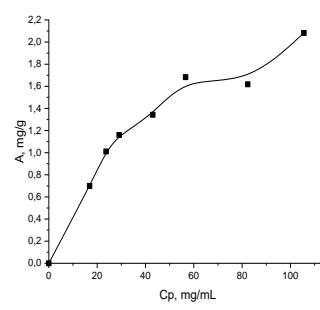
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The goal of this research was to determine the adsorptive characteristics of the surface of magnetite/bicarbonate nanocomposites as to medicinal preparations, which are likely to be practically used in biomedicine.

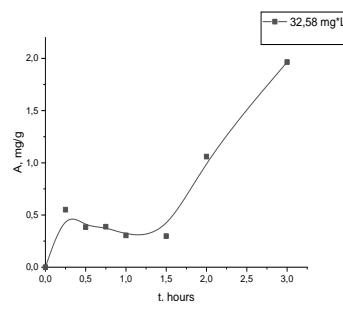
The adsorption of cisplatin (CP) (medicinal preparation of chemotherapeutic action) on the surface of $\text{Fe}_3\text{O}_4/\text{Al}_2\text{O}_3/\text{C}$ has been studied. Herewith, it has been foreseen, that medicinal substances adsorption can be one of the effective ways to create slow-release drugs as well as adsorptive materials. Cisplatin adsorption was studied in static conditions under the temperature of 22–25 °C, with a composite batch ($g = 3 \text{ mg}$, $V = 5 \text{ mL}$). All solutions were prepared adding 0.9 % sodium chloride for creating a constant ionic strength.



Dependence of CP adsorption on pH



Adsorption isotherm of CP ($C_0=21-118 \text{ mg/l}$) on the surface of $\text{Fe}_3\text{O}_4/\text{Al}_2\text{O}_3/\text{C}$



Dependence of CP adsorption on the time on the surface of $\text{Fe}_3\text{O}_4/\text{Al}_2\text{O}_3/\text{C}$

It has been established that the isotherm corresponds to Dubinin-Radushkevych model for CP adsorption from physiological solution with pH=7.

The adsorption kinetics of Cisplatin corresponds to the second-order model ($r^2 = 0.9627$), a limiting factor of adsorption is a film diffusion ($r^2 = 0.9605$).

1. P.P. Gorbyk, N.V. Kusyak, A.L. Petranovska, O.I. Oranska, M.V. Abramov, N.M. Opanaschuk, Him. Fiz. Tehnol. Poverhni. **9** (2018) 176.

Temperature-frequency motion control for a slightly fluctuating ratchet

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Nowadays, creating and controlling nanoparticle transport is an important and interesting problem with large applied potential. We study the ways and mechanisms of frequency-temperature controlling of Brownian ratchet motion. The model is a sawtooth potential of a barrier u_0 and of link widths l and $L-l$, perturbed by the weak spatially harmonic signal $w(x) = w \cos[2\pi(x/L - \lambda_0)]$, the time dependence of which is described by a stochastic dichotomous process. For the extremely asymmetric sawtooth potential ($L-l \rightarrow 0$), an analytical expression for the ratchet average velocity has been obtained. Such a ratchet demonstrates nontrivial behavior as a result of subtle interplay of limiting values of its parameters (asymmetry, frequency, temperature). Analytical and numerical results explain how additional ratchet stopping points can originate from the competition of system characteristic times, when the asymmetry of the sawtooth potential is getting of its limit value; the results also demonstrate the ways to control the motion direction by changing temperature and perturbation frequency values (see Fig.).

This work was supported by the RFBR (projects 20-57-00007_Bel_a and 21-57-52006_MNT_a) and the BRFBR (project F20R-032).

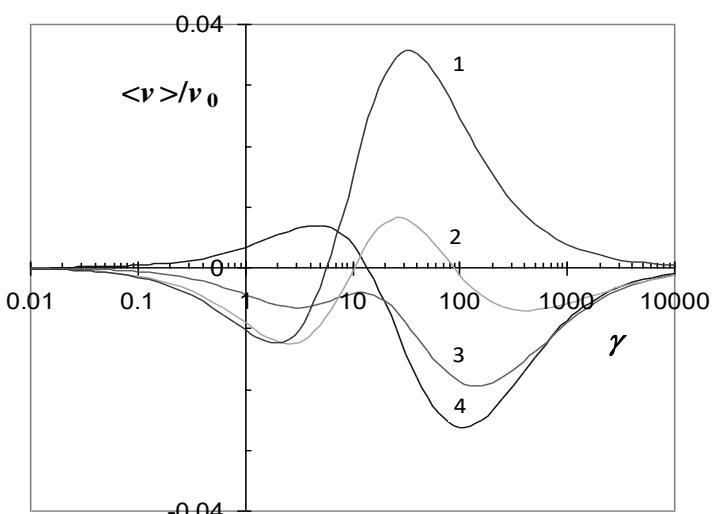


Fig. Frequency dependences of the average velocity at $u_0/k_B T = 5$ calculated for the phase shift $\lambda_0 = 0.29$. The curve numbers correspond to different asymmetries of the sawtooth profile $u(x)$: $l/L = 1$ - exact solution (1), 0.975 (2), 0.95 (3), 0.925 (4)

Unidirectional rotation in a hindered rotation potential

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Brownian rotors (a special case of Brownian motors) convert the energy of an external alternating electric field into the energy of unidirectional rotation in a stationary n -well potential created by a polar substrate. Earlier, we studied a model of a rotor moving under the action of a stationary n -well potential $u(\varphi) = (\Delta u/2)(1 - \cos n\varphi)$, disturbed by a harmonic signal $w(\varphi) = w_0 \cos(\varphi - \varphi_0)$ in the approximation of small fluctuations ($w_0 \ll \Delta u$) [1]. In that work, it was shown that the ratchet effect exists only for $n = 2$ and is forbidden for $n > 2$.

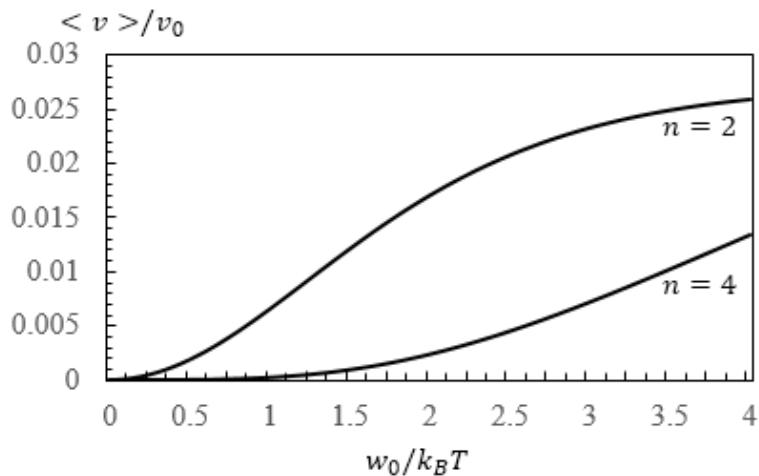


Fig. An average rotor velocity, maximum by phase shift, for $n = 2, 4$ (upper and lower curves respectively), depending on w_0 at fixed $\Delta u / k_B T = 2$

Now we propose a method for calculating the average velocity of a Brownian rotor, which allows one to go beyond the small fluctuation approximation. It is found that for $n > 2$ the ratchet effect exists for an even number of n , and for odd n , it is forbidden due to the fact that the space-time dependence of the potential energy belongs to the class of supersymmetric functions [2]. Fig. shows the w_0 -dependence of the ratchet effect's velocity which is proportional to w_0^n for $n = 2, 4$ at small w_0 . Thus, the calculation performed for an arbitrary ratio of $w_0 / \Delta u$ shows the presence of the ratchet effect for $n > 2$, which was forbidden in the approximation of small fluctuations.

1. V.M. Rozenbaum, O.Ye. Vovchenko, T.Ye. Korochkova, Phys. Rev. E. **77** (2008) 061111.
2. P. Reimann, Phys. Rev. Lett. **86** (2001) 4992.

Game theory description of Brownian motors govern by dichotomous deterministic and stochastic fluctuations

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To simulate the ratchet effect, which can be used to create controlled currents of nanoparticles, nonequilibrium fluctuations usually are implemented into the system by a dichotomous deterministic or stochastic process. The first is typical for artificially created ratchets, in which state switching occurs at fixed time intervals. The second method is inherent for naturally occurring motors (biological molecular motors), driven with random events (for example, conformational molecule changes due to chemical reactions) with average lifetimes of the states.

We have simulated the ratchet effect for a diffusion hopping model of a Brownian motor with an asymmetric double-well on-off potential, using the method of Parrondo's paradox games for both processes controlling motion. It was found that, under otherwise identical values of the systems parameters (i.e. probabilities of particle transitions between wells, temperature, potentials lifetimes), the difference in the way of potential switching plays a very significant role on the occurrence of the ratchet effect. Thus, in the deterministic approach directed motion will be generated only for odd values of discrete potentials lifetimes, while stochastic switching will produce the averaged velocity for any lifetimes values without stopping points (see Fig.).

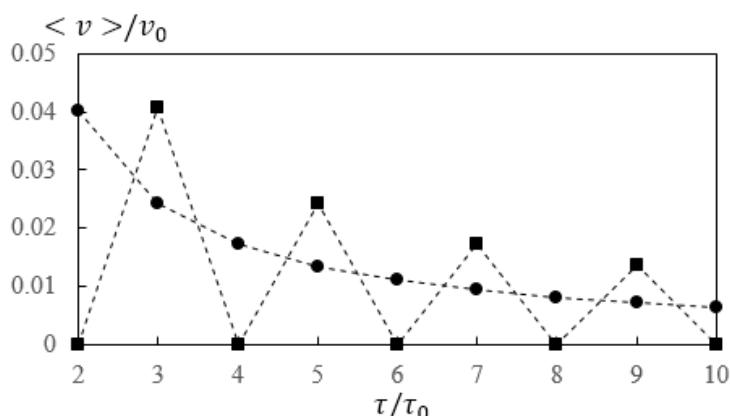


Fig. Dependence of the average particle velocity on the integer lifetime of switching states, square markers correspond to the deterministic version of state switching, and round markers correspond to the stochastic one

Features of Methylene Blue adsorption on Graphene Oxide surface in aqueous medium

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Both Graphene Oxide (GO) nanomaterial and Methylene Blue (MB) dye are among the favourite objects of nanotechnology research and development. Negative charge on oxygen-containing groups of GO and positive charge on MB organic cation facilitate coloumbic attraction and (GO-MB) composite formation. However, the balance of negative and positive charges of the system components may affect the state and stability of (GO-MB) aqueous dispersion.

In the present work the dependences of (GO-MB) aqueous system appearance and UV-vis spectra on the ratio of GO to MB was studied. In the framework of an applied task of GO use as a sorbent for water purification, it may be expected that the increase of GO content would provide more efficient removing of MB (being in some constant concentration) from the liquid phase. It appeared, however, that while the relatively low quantity of GO caused formation of (GO-MB) composite flakes followed by the flakes sedimentation, the excess of GO resulted in preservation of stable dispersion of (GO-MB) composite particles without noticeable separation of the suspension with time. UV-vis spectra shed light on the physical reasons of the phenomenon observed. The shoulder characteristic of MB cations adsorbed in the form of dimers and trimers appeared in the spectra of the systems with MB excess. An expedient of subtraction of the spectrum of the supernatant obtained after a day of storage from the spectrum of just prepared (GO-MB) system permitted us to conclude that the sediment contained GO flakes with MB cations adsorbed at their surface in the form of trimers and higher aggregates. Obviously, the neutralization of the GO charge by intense MB adsorption caused distraction of the suspension and neutral flakes sedimentation. At the same time MB being in low quantity was adsorbed in the monomeric form, as was evidenced by UV-vis spectra; it did not cover the whole GO surface and thus permitted preservation of some part of negative charge on GO flakes and, consequently, preservation of their solubility in water. The novelty of our UV-vis investigations is in evaluation of the composition of the sediments, if formed.

The observed effects are to be accounted during development of GO applications as a pollutant sorbent or a carrier for drug delivery.

Effect of azoinitiators of methyl methacrylate polymerization on phase separation at the formation of polyurethane/poly(methyl methacrylate) interpenetrating polymer networks

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As a rule, the chemical reactions of *in situ* formation of interpenetrating polymer network (IPN) components from single-phase initial mixtures are accompanied by physical process of phase separation due to the incompatibility of the forming components. As a result, heterogeneous systems with big dimensions of phase-separated structures and insignificant interphase adhesion are formed. These systems often have unsatisfactory physicochemical properties. To increase the compatibility of the components and to get structure with smaller dimensions the process of phase separation must be slow down. The rate of phase separation depends on kinetics of the *in situ* formation of the components and on presence of compatibilizers in the system. The purpose of this work is to study the process of phase separation at the formation polyurethane (PU)/poly(methyl methacrylate) (PMMA) IPN in the presence of methyl methacrylate polymerization oligoazoinitiators that contain fragments of a polyurethane chain. The network PU was synthesized from macrodiisocyanate, based on oligo(diethylene glycol adipinate) with MM = 800, hexamethylene diisocyanate and trimethylolpropane. The composition of PU/PMMA was 10/90 by weigh. It has been shown that the process of phase separation takes place in two stages. The nucleation mechanism is preferred at the first stage; the spinodal mechanism is preferred at the second one. The introduction of oligoazoinitiators decreases the rate of phase separation at both first and second stages. It is due to the formation of block copolymers during synthesis, which are compatibilizers of the mixture. They enhance the interaction between the components at the phase boundary and contribute to the formation of a finer IPN structure (Fig.).

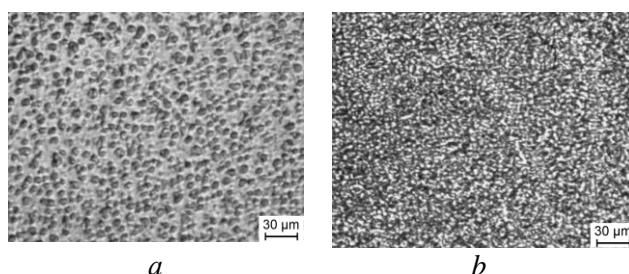


Fig. Microphotographs of IPN without (a) and with oligoazoinitiator (b)

Synthesis of efficient adsorbents by adjusting the spatial arrangement of nanoparticles in iron silicate core-shell composites

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The aim of the work is to adjust the spatial arrangement of SiO_2 nanoparticles in iron silicate core-shell composites by using the bisurfactant template consisting of cetylpyridinium bromide and Tween-80. Specific characteristics of porosity and pore size distribution (PSD) were determined by the method of low-temperature N_2 adsorption-desorption (Fig., Table).

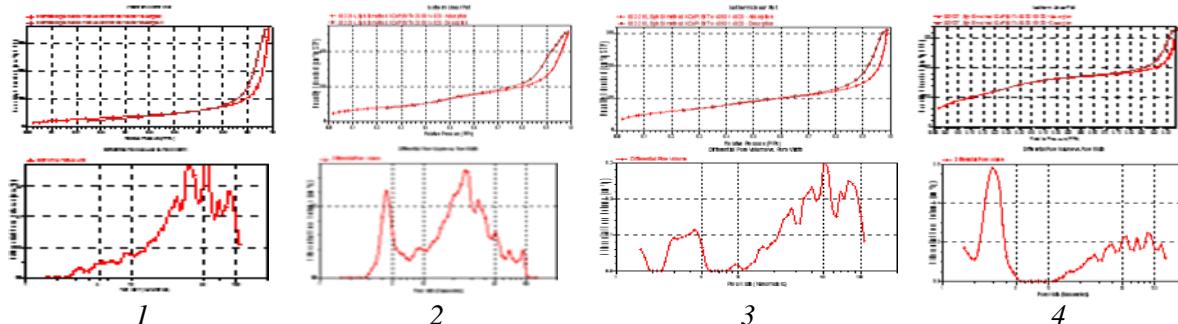


Fig. Isotherms of N_2 sorption and NLFDT-PSD of composites obtained on bisurfactant template with cetylpyridinium bromide / Tween-80 ratio (mol. %): 1 - 0/100; 2 - 20/80; 3 - 40/60; 4 - 80/20

Table. Selectivity and specific characteristics of porosity of iron silicate composites in the reaction of catalytic isomerization of α -pinene epoxide to campholenic aldehyde

№	SAA/ Tween- 80	A_{BET} , m^2/g	$V_{\text{sp des}}$, cm^3/g	Y(I) %	Selectivity, mol. %								
					II	III	IV	V	VI	VII	VIII	VIII	IX
1	0/100	98	0.54	100	43.3	9.2	1.7	6.5	12.8	6.8	8.5	8.5	6.1
2	20/80	220	0.48	100	43.9	8.5	1.9	4.9	15.7	6.9	8.1	8.1	5.5
3	40/60	291	0.78	100	44.9	8.2	2.1	4.3	17.1	8.1	7.3	7.3	3.1
4	80/20	414	0.50	100	51.1	8.0	2.3	3.4	13.0	8.0	7.1	7.1	2.3

Note: Y(I) – conversion of α -pinene epoxide; II – campholenic aldehyde; III – *iso*-campholenic aldehyde; IV – pinocarveol; V – *iso*-pinocamphone; VI – *trans*-carveol; VII – *trans*-sorberol; VIII – *p*-cymene; IX – pinol.

As the cetylpyridinium bromide/Tween-80 ratio increases, the specific surface area and selectivity in the reaction of catalytic isomerization of α -pinene epoxide to campholenic aldehyde also increase (Table). The selectivity changes little despite the fact that some samples have larger specific surface areas. This is because the high surface area can be due to the presence of very small mesopores that are not accessible to large organic molecules (Fig.).

Acknowledgements

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Selective sorption of heavy metals by natural and modified layer silicates

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The separation of mixture of heavy metals with different chemical properties in the effluent is the actual problem, especially for waters of galvanic productions and hydrometallurgical industry. Sorption method is widely used in water treatment technologies because it can provide the lowest levels of residual concentrations of pollutants in water. Cheap natural silicate materials are an alternative to commercially available sorbents (activated carbon, synthetic inorganic sorbents). Modification of the surface of layer silicates with inorganic and organic substances significantly improves their adsorption capacity and selectivity.

The aim of the work is to study the selective sorption of a mixture of heavy metal ions Cu(II), Cd(II), Zn(II), Co(II), Cr(VI) using natural and modified layer silicates.

Studies of heavy metals sorption were performed using natural layer silicates kaolinite (1:1), montmorillonite (2:1), and fibrous silicate palygorskite (2:1). The surface modification of the layer silicates was performed using nanosized zero-valent iron (nZVI). Sodium borohydride (NaBH_4) as reducing agent was used for producing of nZVI. The wastewater that are complex on its content and include a mixture of heavy metal ions (Cu(II), Cd(II), Zn(II), Co(II), Cr(VI)) were investigated.

The specificity of layer silicates as sorbents is due to the presence of two types of active centers located on the basal and edge surfaces of clay particles. The sorption values of heavy metal ions on the surface of the natural layer silicates differ significantly: sufficiently high values for copper(II) ions and almost close to zero for chromium(VI) ions. The sorption centers $>\text{S} - \text{OH}$ on surfaces of layer silicates form strong complexes with heavy metal ions, which correspond to the Irving-Williams series of stability of the corresponding complexes in solutions: $\text{Cu} > \text{Zn} > \text{Co} > \text{Cd} > \text{Cr}$. The values of sorption of heavy metal ions by modified nZVI layer silicates at pH 6 are several times higher than the values for natural ones. The extraction of Cr(VI) from solutions occurs by two parallel mechanisms. The first one is sorption of the anionic form of chromium on active centres of hydroxide film which formed on the surface of iron nanoparticles due to their partial oxidation (so-called “core-shell” structure). The second one is reduction of Cr(VI) by nanodispersed zero-valent iron to the lower valent state.

Interfacial properties of chitosan lactate at the liquid/air interface

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The interfacial properties (dynamic and equilibrium surface tension, viscoelasticity modulus) of chitosan lactate were studied at the liquid/air interface by the oscillating drop shape method at (25 ± 0.1) °C. Chitosan with a molecular weight of 75 kDa and a degree of deacetylation of 70 % was used in this work. Solution of chitosan lactate was prepared by dissolving chitosan in an 2 % aqueous lactic acid solution. The pH of the resulting solution was 4.0.

The equilibrium surface tension decreases with an increase in the concentration of chitosan to 1.0 g/L, after which it remains almost constant. Such constant level of surface tension can be explained by changes in the surface layer structure (two-dimensional condensation of molecules) or multilayer formation. Chitosan is a weak cationic polyelectrolyte which can change its conformation from a linear line to a chaotic and compacted coil. Therefore, the experimental dependence of the equilibrium surface tension on concentration of chitosan lactate was analyzed from the standpoint of the nonideal two-dimensional solution model proposed for proteins in [1, 2]. Good agreement between the calculated and experimental values of surface tension was observed.

The study of the rheological characteristics of the formed adsorption layers of chitosan lactate reveals that the dependence of the surface viscoelasticity modulus is extreme in nature with a pronounced maximum at a concentration near 0.7 g/l. This is due to the possibility of changing the molar surface area of the polyelectrolyte at the interface depending on the amount of adsorption and its structural properties. An attempt to theoretically describe the viscoelasticity modulus within the framework of model [1, 2] accounting mono- or bilayer adsorption did not lead to a satisfactory result. This may be due to barrier adsorption mechanism of chitosan. The values of the surface viscoelasticity modulus of chitosan lactate occupy an intermediate position in comparison with the data available in the literature for globular and flexible-chain proteins, that is consistent with their molecular structure.

1. V.B. Fainerman, R. Miller, Colloid Journal. **67** (2005) 393.
2. V.B. Fainerman, E.H. Lucassen-Reynders, R. Miller, Adv. Colloid Interface Sci. **106** (2003) 237.

Influence of Cr³⁺ and Fe³⁺ chelate complexes on nitroxyl spin probe penetrability into polymer blend/CNT/Ni nanocomposite

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Previously in [1] the influence of metal coordination complexes was demonstrated on the EMI-shielding characteristics of incompatible polymer blend of cross-linked polyurethane and linear polymethyl methacrylate filled *in situ* with conductive and/or magnetic filler. In addition, the introduction *in situ* of small amounts of nano- and micro-sized fillers into the composite can influence the polymer packing. In this work the influence of Cr³⁺ and Fe³⁺ chelate compounds is analyzed on nitroxyl spin probe penetrability into polymer matrix formed in the presence of from 1.5 to 3.0 % carbon and Ni fillers.

The permeability of nanocomposites was investigated by EPR method using proportionality of TEMPO spectrum intensity (I) to the number of paramagnetic centers penetrated into the sample. It was revealed significant increasing of permeability of composites formed in the presence of Fe(acac)₃ compared to the unfilled polymer blend indicating the loosening of polymer matrix (Fig. a). The opposite tendency is observed for Cr(acac)₃-modified composites that are more packed as compared to unfilled blend (Fig. b).

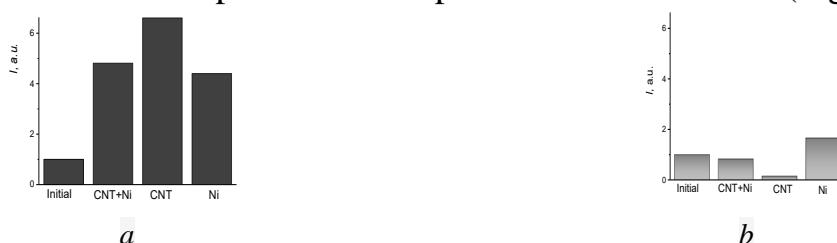


Fig. Relative integral intensity (I) of TEMPO spectra in composites and unfilled polymer blend, modified with Fe(acac)₃ (a) or Cr(acac)₃ (b)

It is also noteworthy that the permeability of the probe in the CNT-filled blend modified with Fe(acac)₃ is the highest, whereas in the similar systems modified with Cr(acac)₃ it is the lowest. Compared to CNT-filled composites, the Ni filler partially seals the Fe(acac)₃-modified polymer and loosens the Cr(acac)₃-modified polymer.

The results obtained indicate that the introduction *in situ* of small amounts of nano- and micro-sized fillers in the polymer composite is able to significantly affect the structure of the polymer and is sensitive to the presence in the reaction mixture of active complexing dopants.

1. N. Kozak, L. Matzui, L. Vovchenko *et. al.* Composit.Sci.Technol. **200** (2020) 108420

Polylactide-silica composites for biomedical application with controlled release of active agents

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Biodegradable natural polymers have many medical applications in controlled delivery systems active substances. In recent years, many efforts have been made to the development of new polymer materials from renewable resources. Among the biopolymers used in medical and pharmaceuticals industries these days, polylactide (PLA) is considered as one of the best materials. The formation of nanocomposites based on hybrids of an organic matrix and inorganic materials can show improved characteristics. This work is devoted to the development of synthesis methods and the study of properties of composites in which the base is silica and aminosilica, and the main function of the polymer matrix is performed by polylactide (PLA). The production of composite materials was carried out by polymerization of *L*-lactide with the opening of its ring in the surface layer of a silica. Obtained materials were characterized by FTIR, TG and tested *in vitro* release active components. Active ingredient of diclofenac sodium (99.5 wt.%, Vaishali Pharmaceuticals, India) and ibuprofen (98.5 wt.%, Sigma-Aldrich) was used as received. Immobilization of the active component on polylactide-silica composites was performed by mixing of 1 g of carriers with 1.5 mL of ethanol solution of diclofenac sodium or ibuprofen (50.0 mg/mL). After impregnation for 24 h the drug-loaded materials were filtered and dried at 80 °C for 3 h. *In vitro* release studies of the prepared biocomposites were executed according to the requirements of the State Pharmacopoeia of Ukraine by the rotating basket method. The active agent concentrations in the release liquids were registered spectrophotometrically by measuring the increase in absorbance at 230 nm for ibuprofen (Fig. 1) and diclofenac at 276 nm (Fig. 2).

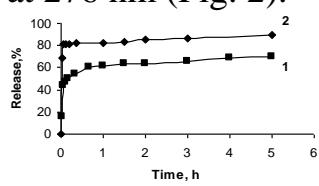


Fig. 1. Release of ibuprofen from composites Silica/PLA (1) and Silica-NH₂/PLA (2)

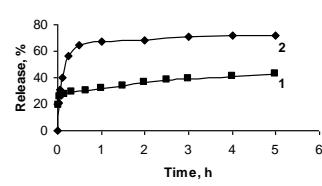


Fig. 2. Release of diclofenac from composites Silica/PLA (1) and Silica-NH₂/PLA (2)

Release of active agents was demonstrated to depend on the different surface functionalities of the silica carriers in the polylactide-silica composition.

Synthesis and sorption capacity of lignin modified with nanodispersed iron oxide with respect to radionuclides

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The development of new sorption materials capable of selectively sorbing radionuclides from aqueous media is an important task of modern radiochemistry. To increase the efficiency and selectivity of radionuclide extraction, various methods of modifying natural materials are used, as they are an affordable and cheap raw material base. It should be noted that the vegetable raw materials, which is used to obtain composite materials, after modification, may have high sorption properties that exceed inorganic sorbents.

Hydrolysis lignin is a cheap, non-toxic material that is a product of softwood processing and contains a large number of active functional groups, making it quite easy to chemically modify it. However, such sorbents, as a rule, have low kinetic characteristics and relatively low sorption capacity.

In this work, a sorption material based on hydrolyzed lignin modified with nanodispersed iron oxide Fe_3O_4 was obtained and the sorption capacity of ^{137}Cs , ^{90}Sr and ^{60}Co radionuclides was studied.

The introduction of $\gamma\text{-Fe}_3\text{O}_4$ particles into lignin forms a chemical bond of iron oxide particles with lignin functional groups. This modification contributes to a significant improvement in the sorption properties of the sorption material.

The optimal content of the modifier in the sorption material for maximally efficient extraction of radioactive isotopes from aqueous solutions consists by 10-50 % of the weight of the sorbent.

Sorption capacity was studied by the method of limited volume in the range of pH values from 2 to 9 at the temperature of 293 K.

The sorption of radionuclides is minimal at pH = 2 and increases with increasing of pH.

Analysis of the obtained kinetic curves of radionuclide sorption on the investigated sorbent showed that the sorption equilibrium in the radionuclide-sorbent systems occurs after 2 hours.

The analysis of the obtained data showed that the modified lignin by its sorption capacity exceeds the hydrolysis lignin by almost 2 times.

Protein adsorption and hemostatic properties of composite materials based on highly dispersed silica and sodium alginate

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Trauma-induced hemorrhagic shock is the leading cause of death during hostilities and the second most common cause of death in civilian traumatology clinics. Therefore, the creation of effective hemostatic materials remains a topical problem. In this work, a new composite material with extraordinary hemostatic ability was obtained by combining the cellular structure of polyurethane foam with water-absorbing, osmotic and protein adsorption properties of highly dispersed silica and sodium alginate.

The composites were prepared by soaking polyurethane foam (PUF) in 1 % solutions of sodium alginate (Alg-Na) with the addition of 5 % or 10 % silica A-300, followed by drying at a temperature of 70 °C. It was found that the highest indexes of both osmotic activity and water absorption has a sample with a silica content of 5 wt.%. The specific surface area of the samples synthesized by drying 5 % aqueous suspensions of A-300 corresponds to the specific surface area of the initial silica and decreases slightly with increasing Alg-Na content. However, the ability of such samples to adsorb gelatin is significantly reduced compared to the initial A-300 and depends little on the addition of Alg-Na. Infrared spectroscopy showed that in samples containing Alg-Na, significant perturbation of silanol groups does not occur, i.e. the surface of silica remains available for interaction with protein molecules.

In a model of parenchymal bleeding from rat liver, it was shown that composite materials based on PUF, which contain silica and sodium alginate, have a pronounced hemostatic effect. Thus, the lowest values of blood loss (about 0.12 g) were observed using “PUF / Alg-Na 1 %” composite, as well as (about 0.15 g) when using “PUF / Alg-Na 1 % / SiO₂ 5 %” composite. For comparison: blood loss when using a commercial analogue was 0.23 g, while the application of medical gauze as a control leads to blood loss up to 0.75 g.

Reactive-landing of nickel(II) tartaric acid complexes on self-assembly monolayer surfaces for catalytic applications

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Soft and reactive landing of mass-selected ions as well as the nanoparticle beam deposition are considered as advanced ways to the creation of novel high-selective heterogeneous catalysts [1, 2]. Mass-selected ion deposition offers several unique advantages for obtaining a molecular-level understanding of interactions of complex molecules with surfaces [3]. This study was devoted to the reactive-landing of mass selected organometallic chiral complexes to the surface of functionalized thiols. The preparation of carboxy-terminated thiol self-assembled monolayers was done on the gold substrates. The gas-phase chiral complexes of nickel(II) tartaric acid were prepared *in situ* via electrospray ionization. Reactive landing of the organometallic complexes was performed and confirmed by simultaneous IR experiment. SIMS was used for further characterization of samples.

Soft-landing experiments were performed using a custom-designed soft-landing instrument equipped with a high intensity electrospray ionization source and a quadrupole mass filter. Charged droplets produced by ESI are dried in a heated inlet maintained at 150 °C and transferred into the vacuum system through an electrodynamic ion funnel followed by a collisional quadrupole. Mass-selected ions are deposited onto a surface positioned after the mass filter. Ion current on the surface is monitored using a picoammeter. SIMS analysis was performed using a commercial PHI TRIFT II TOF-SIMS instrument (Physical Electronics, Eden Prairie, MN). IRRAS experiments were performed using a Vertex 70 FTIR spectrometer (Bruker Optics, Billerica, MA).

Acknowledgements

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Carrier systems for anticancer drug on the base of double hydrophilic block copolymers

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The application of micelle-type polymeric nanocontainers is considered as one the most perspective ways to realize a targeted delivery of toxic and/or water-insoluble drugs into certain cells of living organisms. It was shown earlier that the asymmetric diblock and triblock copolymers comprised chemically complementary (methoxy)poly(ethylene oxide)/polyacrylamide ($\text{DBC}_{\text{MOPEO/PAAm}}$ and $\text{TBC}_{\text{PEO/PAAm}}$) and partially hydrolyzed triblock copolymer derivative ($\text{TBC}_{\text{PEO/P(AAm-co-AAc)}}$) formed unusual micellar structures in aqueous solutions. The ability of these micelles to encapsulate a toxic anticancer drug doxorubicin (Dox) and to enhance its cytotoxicity as compared to pure Dox has been discovered [1, 2].

Later, in search of the effective micellar nanocontainers for poorly soluble and/or toxic drugs, we synthesized two series of asymmetric block copolymers comprised poly(acrylic acid) blocks with constant chain length and polyacrylamide blocks with variable chain length ($\text{DBC}_{\text{PAAc/PAAm}}$ and $\text{TBC}_{\text{PAAc/PAAm}}$) using RAFT/MADIX controlled radical polymerization. The special micellar properties of mentioned block copolymers in aqueous medium has been proved [3].

In the present work, we studied the encapsulation capability of $\text{DBC}_{\text{PAAc/PAAm}}$ and $\text{TBC}_{\text{PAAc/PAAm}}$ micelles with respect to Dox by the methods of static light scattering, FTIR, UV-Vis, TEM and examined a biological action of the drug/micelles compositions on cancer cells. The dependence of Dox encapsulation degree on the length of the corona forming PAAm blocks and the solution pH was established. $\text{DBC}_{\text{PAAc/PAAm}}$ micelles were shown to encapsulate Dox more effectively as compared to $\text{TBC}_{\text{PAAc/PAAm}}$ ones. The results of biological tests carried out against the cells of human T-leukemia indicated a high cytotoxicity of both created micellar systems with the drug. Thus, a real prospect for their possible application in the cancer therapy was opened.

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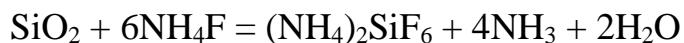
Ammonium fluoride technology for producing amorphous silicon dioxide nanopowders from industrial waste

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The aim of this work is to develop a technology for producing amorphous silicon dioxide nanopowders with specified properties. Slags from the copper-smelting industry of the Almalyk Mining and Metallurgical Combine and silicon production waste - silica fume - were used as initial materials.

For the synthesis of amorphous SiO_2 nanoparticles, a fluorinating reagent, crystalline ammonium fluoride (NH_4F), was used. The process of obtaining SiO_2 nanoparticles includes sintering the initial material with NH_4F at temperatures of 90-160 °C until a powder pitch is formed, then the resulting mixtures of fluoroammonium compounds of Si are processed at temperatures of 320-400 °C to sublime ammonium hexafluorosilicate ($(\text{NH}_4)_2\text{SiF}_6$):



SiO_2 powders are obtained by hydrolyzing $(\text{NH}_4)_2\text{SiF}_6$ under the action of ammonia water.

Figure shows the resulting typical three-dimensional size distribution of synthesized SiO_2 nanoparticles.

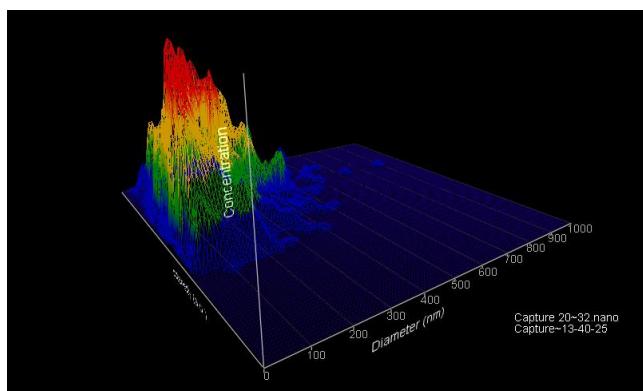


Fig. Three-dimensional size distribution of synthesized SiO_2 particles

It is shown that the sizes of SiO_2 nanoparticles depend on the concentration of ammonium hexafluorosilicate in solution and the temperature at which hydrolysis occurs. It was found that the size distribution of synthesized SiO_2 nanoparticles can also be controlled by the fractional composition of the initial material.

The range of distribution of nanoparticles synthesized from microsilica is 15-300 nm, while from slags of copper-smelting production - 40-450 nm. Moreover, most of the particles (90 %) have a diameter of 40-200 nm. The purity of the obtained powders for SiO_2 is not less than 99.97 % of the mass.

Potentiometric titration as efficient method to characterize acidic properties of hierarchical zeolites

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Hierarchical zeolites are new class of zeolite materials combining micropore and mesopore structure which facilities transport of bulk molecules to active site and let improve catalytic properties in process including them. To predict catalytic properties of such materials it is necessary to know their acidic or basic properties including type, concentration and strength of active sites. Hierarchical zeolites were synthesized using Gemini-type surfactants as structure directing agents synthesized by the method proposed by Ryoo [1]. Acidity of hierarchical zeolites were investigated by potentiometric titration. pK_a of samples was calculated by Gran theory [2]. It was established that the strength of Bronsted acid sites (BAS) within one zeolite structure (BEA, MTW, MFI) decrease in the range Al> Ga >> B, but the difference in the strength of the centers of aluminosilicate and germanosilicate centers is not significant. For aluminosilicate zeolites the strength of BAS increases in the following range BEA < MFI < MTW < MOR (see Fig.).

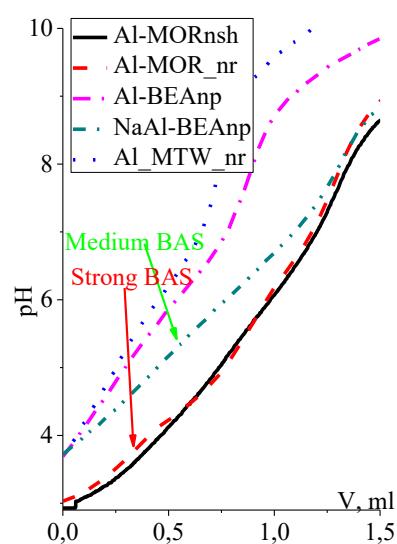


Fig. Typical curves for potentiometric titration

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Dehydration of 4-bromo-2,3-dihydro-1H-inden-1-ol on hierarchical zeolites

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Indene are an important component of indene/coumarone thermoplastic resins and it is widely used in industry. Lately, different indenes are widely used as ligands for new type stereoselective catalysts for α -olefines polymerization. Typical method for their production is dehydration of corresponding indenols using different homogeneous acid catalysts which are complicated by undesirable reactions such as formation of dimers and polymerization of obtained indenes. Due to high concentration of active sites available for bulk molecules and developed external surface, hierarchical zeolites are promising catalysts for a variety of catalytic process. B-, Ga- and Al-containing hierarchical zeolites were obtained using different Gemini-type surfactants as structure-directing agents (SDA). Significant decrease in particle size allow to increase values of external surface area and mesopore volume values of which achieved up to $600 \text{ m}^2 \cdot \text{g}^{-1}$ and $1.4 \text{ cm}^3 \cdot \text{g}^{-1}$, consequently. Zeolites possessed a high concentration of Brønsted (BAS) and Lewis acid sites (LAS) ($50 - 400 \mu\text{mole} \cdot \text{g}^{-1}$) available for bulk molecules, fraction of which is achieved 85%.

Catalytic activity of hierarchical zeolites was investigated in 4-bromo-2,3-dihydro-1H-inden-1-ol dehydration process (Fig.). B-, Ga-, Al-containing zeolites provide high catalytic activity in this process and 100 % indenol conversion was achieved. For Ga- and B-containing hierarchical zeolites due to high fraction of weak and medium BAS high selectivity to corresponding indene was achieved (selectivity >96 %, complete conversion). Selectivity of hierarchical zeolites decreased with increase of BAS strength in following order B-BEA < Ga-BEA < Al-BEA.

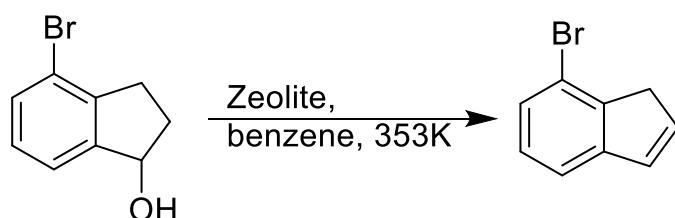


Fig. Dehydration of 4-bromo-2,3-dihydro-1H-inden-1-ol

Synthesis and properties of antibacterial materials based on bioactive glass 60S

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The use of bioactive materials as auto-bone substitutes, including various types of sol-gel glass (BG), can solve the problem of the most serious complications associated with endoprosthesis - the problem of infection, as the antibacterial component is released at the site of action, increasing local concentrations, with minimal or no systemic toxicity. The potential of BG as a delivery system of biomaterials for antimicrobials is studied mainly in three areas [1]. One of them is based on the release of ionic compounds when BG is dissolved, resulting in a local increase in pH, increased salts concentration and osmotic pressure, thus creating an unsuitable environment for bacterial growth and preventing the formation of pathogens biofilm production.

The second way involves doping BG during its synthesis of biocidal metals (Ag, Ga, Cu, Zn). Three typical BG doping methods are used: by adding a compound during glass melting or sol-gel synthesis, or by incorporating certain ions into the glass structure by ion exchange processes. During the dissolution of BG ions included in its structure are released into the environment and inhibit the growth of bacteria.

The third way involves the delivery of antibiotics from the surfaces of BG or from the polymer phase. Given the internal nanopores and high surface area, the simplest way to prepare BGs carriers is the vacuum infiltration method. However, such systems have a limited ability to control the rate of antibiotic release. Another alternative developed for BG-based materials as a drug delivery system is based on antibiotic-loaded biopolymer films in which BG particles are dispersed. The present work discusses peculiarities of synthesis of materials based on bioactive glass 60S and antibiotic Vancomycin, their properties and prospects of application as an implant material with the function of drug delivery with therapeutic properties and prolonged action for topical use [2].

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Synthesis and properties of nanodisperse luminophores for photodynamic and optopharmacologic therapies of tumors of cranial cavity and bone tissue

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Developing of multifunctional drugs enabling targeted delivery and metered local release of bioactive components is outstanding problem of modern pharmacology and medicine. For oncology, the concept of chemical design of magnetosensitive core-shell-type nanocomposites with a multilayered hierarchical shell nanostructure capable of performing the functions of medical-biological nanorobots has become a priority [1]. Aside of precise delivery and deposit of drugs in target cells and organs, these functions may also include recognition of pathogens in biological environments, local chemo-, immuno-, neutron-capture-, hyperthermic- and photodynamic therapies, real time magnetic resonance imaging diagnostics, detoxification of the body by adsorption of cells' degradation products, viral particles, heavy metal ions, etc. and their removal by magnetic field [1]. In onco-orthopedic surgery, it is important to develop new types of implants for the use as comprehensive local delivery system for chemotherapeutic and osteoconductive drugs with prolonged action [2].

Among new approaches that may be useful for treatment of minimally invasive, malignant tumors localized in the cranial organs, bone tissue, and other deep tissue layers may be photodynamic therapy and optopharmacology in combination with X-ray irradiation. The present work discusses peculiarities of synthesis of nanodisperse phosphors based on lanthanum fluoride and lanthanum phosphate, their properties and prospects of application in photodynamic and optopharmacological therapy of tumors of cranial organs and bone tissues under conditions of irradiation by "soft" X-ray.

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IR spectroscopic study on peculiarities of fumed silica hydridesilylation with triethoxysilane under fluidized bed conditions

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Fumed silica has found widespread application in industry due to variety of fascinating properties. Owing to its specific manufacturing process it consists of finely dispersed particles and featured with large specific surface area covered by profoundly reactive silanol groups which are available for chemical grafting. Spherical shape of fumed silica particles and lacking porosity provides a space-filling structure. These characteristics implement the fumed silica's utilization as high-surface-area fillers and carriers for various catalysts, i.e. metallic nanometer-sized particles, organic moieties and *etc.* Currently, a great attention is called to on-surface grafting to improve the silica-based carrier strength. Most of research is carried out in area of wet-chemistry involving an abundance of expensive and often toxic solvents while the space-filling properties of silica is favoring reactions under fluidized bed conditions.

In current research fumed silica (A-300) was a subject for hydridesilylation with triethoxysilane under fluidized bed conditions to improve a resulting carrier loading capacity. In all synthesis reported in current research the insignificant amount of solvent (1.00 wt.% of the amount used in typical wet-chemical modifications method) was spent in order to dissolve modifier and catalyze the silanol surface grafting. While the mass ratio of silica/modifier was kept constant, other conditions, i.e. solvent/catalyst presence, surface pretreatment, presence of water in the system, and the fluidized bed heating mode were varied.

FTIR spectroscopy revealed the interaction between alkoxy groups of triethoxysilane and the silanol groups of the silica, confirmed the presence of grafted silicon hydride groups, and demonstrated the effect of modification conditions on reaction completeness. Scanning electron microscopy and low-temperature nitrogen adsorption studies have shown only slight effect of fluidized bed mode of silica modification on its structural characteristics, including specific surface area and morphology of aggregates, while thermogravimetric analysis demonstrated that surface silicon hydride groups in the resulted modified silica are indeed chemically grafted to its surface.

Catalytic properties of ZnO/MgO-SiO₂ systems in ETB-process: Effect of composition

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Nowadays the design of high active and selective catalysts for the ethanol-to-butadiene (ETB) process, especially using of ethanol-aqueous mixtures as a feed, is one of actual directions of sustainable chemistry related with the development of the technologies based on bio-raw materials for large-volume chemical processes [1].

The purpose of this work is to study the effect of composition on the acid-base surface characteristics of ZnO/MgO-SiO₂ systems and their catalytic properties in the conversion of aqueous ethanol into 1,3-butadiene (BD).

Three-component oxide samples of ZnO/MgO-SiO₂ with various MgO:SiO₂ ratios (1:1 – 3:1), also ZnO/MgO and ZnO/SiO₂ have been prepared and characterized by temperature-programmed desorption of CO₂, NH₃ and H₂O, FTIR spectroscopy with adsorbed pyridine and CO₂, temperature programmed surface reaction of ethanol and isopropanol, and reaction of isopropanol conversion. The effect of MgO:SiO₂ ratio in the catalysts on catalytic performance in 1,3-butadiene production from aqueous ethanol have been investigated. The results indicate that hydrophilicity of ZnO/MgO-SiO₂ is determined by MgO:SiO₂ ratio, and the chemisorption of water molecules occurs preferably on Mg-containing sites. The presence of water in the initial ethanol leads to a decrease in formation of C-C coupling products. The hydrated sites formed in the interface of magnesia and silica remain active in C-C coupling reaction even in the presence of water.

The selectivity of BD formation > 60 % is achieved in the conversion of ethanol-water mixture (80 vol.% ethanol) in the presence of ZnO/MgO-SiO₂ catalysts with the ratio of MgO:SiO₂ = (1:1) and (3:1) [2,3].

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Design and computational study of an all-carbon water desalination membrane

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We present a previously unexplored design of an all-carbon membrane for reverse osmosis—based water desalination and employ computer modeling to gain insight into the structure of the membrane needed to achieve the best permeability and selectivity.

The proposed membrane represents a layered structure containing aligned graphite oxide flakes in its core, sandwiched in-between layers of buckypaper and carbon fibers. This assembly provides thermal stability, resilience to harsh chemicals and mechanical impact, thus responding to multiple challenges that cannot be solved using conventional polymer membranes.

Using *ab initio* DFT calculations we have modeled the permeation of water molecules and hydrated ions through layered graphite oxide. 7 Å-wide edge pores provide the best salt rejection, while maintaining good water permeability. Termination of the graphene oxide edges with hydrogen atoms allows for the best permeation ratio between hydrated ions and water molecules. The hydrophilic surface of graphene oxide slows down the movement of ions along the layers, thus providing for additional salt rejection. We corroborate the possibility of concerted passage through in-layer pores, a mechanism that is accessible to water molecules but not hydrated ions.

The results of our modeling show that the optimized structure of the all-carbon membrane may turn out to be the next step in the design of advanced reverse osmosis membranes.

Silica-based polystyrene-acrylic hybrids as cationic dyes adsorbents

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Organic-inorganic hybrid materials were prepared by the one-step sol-gel method from tetraethyl orthosilicate (a silica source) and styrene-acrylic polymer Tubifast 4010® (SAP). Three hybrids with various ratios SiO₂-SAP1 (5/1), SiO₂-SAP2 (10/1), and SiO₂-SAP3 (20/1) were synthesized and their application for dyes removal was investigated. The structure and properties of the obtained samples were examined by elemental analysis, electrokinetic potential measurements, IR spectroscopy, low-temperature nitrogen adsorption-desorption, SEM, and EDXS analysis (see Table). The synthesized materials are mesoporous matrices with carboxyl and phenyl groups and their isoelectric point values are in the acidic region making it possible to use them as adsorbents for cationic dyes, such as Methylene blue (MB) and Rhodamine 6G (R6G). The adsorption efficiency was determined by the difference in the concentration of dyes before and after contact of the adsorbents with the solutions at pH=7 for 24 h, these concentrations were investigated by UV-visible spectrophotometry for MB ($\lambda_{\text{max}}=665$ nm) and R6G ($\lambda_{\text{max}}=527$ nm). The mechanisms of interaction of hybrids and dyes (physical and chemical) may be different and they are still being studied. Thus, the described materials may be regarded as effective adsorbents for the removal of Methylene blue and Rhodamine 6G from aqueous solutions among another silicas.

Table. Composition and properties of the hybrids

Sample	Elemental analysis data, mass.%		pI	S_{sp} , m ² /g	V_{total} , cm ³ /g	d_{BJH} , nm	Dyes uptake from 50 mg/l solution, mg/g	
	C, %	H, %					MB	R6G
SiO ₂ -SAP1	15	3.0	35.2	2.8	399	0.824	6.6	32.3
SiO ₂ -SAP2	9.5	2.7	41.6	2.7	497	0.850	5.7	31.5
SiO ₂ -SAP3	5.3	2.2	44.7	2.6	548	1.049	6.6	12.7

Acknowledgements

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Antioxidant and antimicrobial properties of the composite comprising of caffeic acid and fumed silica

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Fumed silica is biocompatible and bioactive powder used as an auxiliary ingredient for preparation of the medicines and dietary supplements. The role of silica in such the formulations is to improve the stability of the active components against oxidation, to reduce their hygroscopicity, to introduce hydrophobic compounds into aqueous solutions and hydrophilic compounds into lipophilic media. In some cases, its inclusion in the composite can also decelerate the release of bioactive compounds into solution, thus providing their prolonged action. In this work we prepared the composite of fumed silica with caffeic acid and studied antioxidant and antimicrobial properties of caffeic acid both in the composite and in the solution.

A300+CA composite of fumed A300 silica with caffeic acid (CA) was obtained using the sorptive modification of silica with CA solution. Antioxidant properties of the CA solution and the A300+CA composite containing the same CA amount were tested in the reactions with DPPH[•], OH[•] and NO[•] radicals. Antimicrobial activities of the CA solution and the A300+CA composite were examined using test culture of *Staphylococcus aureus* 209.

The results have shown that caffeic acid is an effective antioxidant, with each molecule of caffeic acid rapidly inhibiting 4-5 molecules of DPPH radical. In the case of the A300+CA composite, the scavenging of DPPH[•] radicals during the first hour proceeded slower comparing to the CA solution, but in several hours the residual concentration of radicals in the reaction mixture was the same as for the CA solution. The CA solution and the A300+CA composite also had a similar activity as NO[•] radicals scavengers and as antimicrobial agents; on the other hand, the CA solution was more effective in inhibition of OH[•] radicals. The similarities and distinctions in bioactivity of the CA solution and the A300+CA composite are consistent with the data on desorption of caffeic acid from the composite into solutions. In the case of very reactive OH[•] radicals, the rate of CA desorption is not sufficient to scavenge all OH[•] radicals. In all other cases, the gradual release from silica surface was a positive factor that provided prolonged action of caffeic acid as antioxidant and antimicrobial agent.

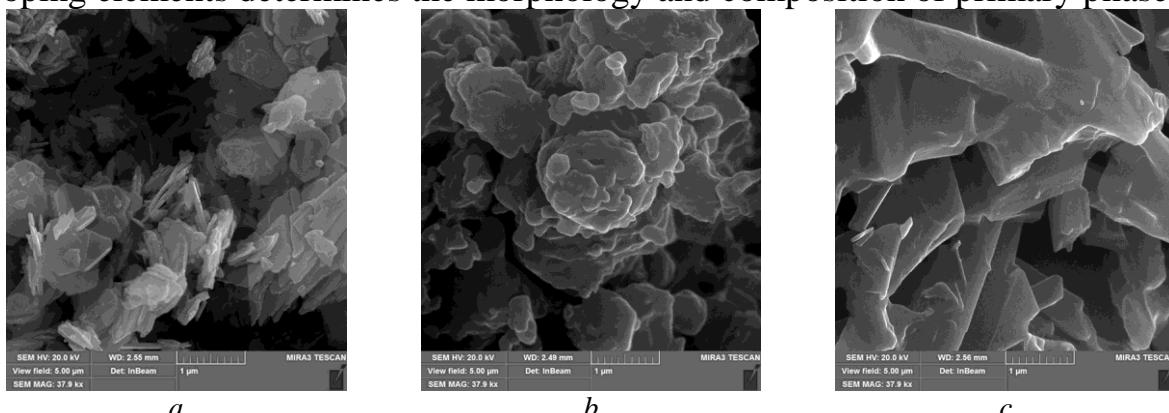
Morphology of primary phases used to obtain functional composites based on rare earth oxides doped with silver

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Nanoscale composites based on rare earth oxides modified with various noble metals, including silver, are considered as attractive materials for technical and biomedical applications due to the combination and improvement of their individual intrinsic properties. It is well known that the synthesis procedure strongly affects on the structure, phase, and prepared nanomaterials' chemical composition. In this case the nucleation mediate stage and primary (precursor) phases' growing can be indicated as the main aspect to form homogeneous materials with controlled physical-chemical properties.

This work makes showing the morphology of the precursor phases used to obtain silver-doped cerium and lanthanum oxides possible. The synthesis of the primary phases was carried out by gradual precipitation of cerium nitrate and lanthanum sulfate with silver nitrate in an alkaline medium under controlled hydrolysis conditions. Whereas the hexagonal crystals $\text{La}(\text{OH})_3$ belonged to $P\bar{6}_3\text{m}$ space group (Fig. a) and the plate like 2D crystals of $\text{Ce}(\text{OH})_3$ (Fig b) are formed in the presence of 4 wt.% AgNO_3 , the addition of $\text{Ce}(\text{NO}_3)_3$ leads to change in the morphology of lanthanum hydroxide (Fig. c). The average chemical composition of $\text{La}(\text{OH})_3$ according to EDS-data includes wt.%: 63 – La, 24 – O, and 13 total N, S, K, but Ag is undetectable. The EDS spectrum of $\text{Ce}(\text{OH})_3$ shows, wt.%: 66 – Ce, 3.8 – Ag, 23 – O, and 7.2 – N. The composition of $\text{La}(\text{OH})_3$ formed in the presence of Ce^{3+} is the following, wt.%: 47 – La, 5 – Ce, 35 – O, and 13 – total N, Na. Therefore, the nature of rare earth species and doping elements determines the morphology and composition of primary phase.



**Fig. SEM images of the precursor phases: a – $\text{La}(\text{OH})_3$ doped with Ag^+ ;
b – $\text{Ce}(\text{OH})_3$ doped with Ag^+ ; c – $\text{La}(\text{OH})_3$ formed in the presence of Ce^{3+}**

Hierarchical nitrogen-doped multi-walled carbon nanotubes as new nanomaterial

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Due to chemical inertness, anomalous strength, high specific surface area and ordered structure multi-walled carbon nanotubes (MWCNTs) show themselves as promising material for many fields [1]. Hierarchical multi-walled carbon nanotubes (h-MWCNTs) is new and poorly studied material. They are consist of the nanotubes with smaller diameter (secondary nanotubes) located on the surface of the MWCNTs of larger diameter (initial nanotubes) [2]. Their branched ordered structure result in higher specific surface area, catalytic activity and electrical conductivity compared to ordinary MWCNTs. These factors make their application attractive as catalysts and components of electronic systems [2, 3]. Obtaining h-MWCNTs doped by nitrogen atoms (h-N-MWCNTs) is an urgent task because nitrogen atoms can donate additional pairs of electrons to the π system of graphene layers. It is result in enhancement in their electronic properties and chemical reactivity [4].

In this work, we for the first time have synthesized h-N-MWCNTs by the catalytic CVD decomposition of acetonitrile over Co-based nanoparticles and have studied their structure and electrical properties. Results shown that mean outer diameter of initial nanotubes equals to 50 nm, while the outer diameters of secondary ones are in the range of ~10-20 nm. h-N-MWCNTs are characterized by the absence of impurities and damages, high defectiveness ($ID/IG = 1.4$) and presence of pyridinic, graphite and pyridinic N-O nitrogen atoms embedded into carbon framework. The studied sample of h-N-MWCNTs shows semiconductor behavior ($dR/dT < 0$) in wide range of temperatures (4.2–300 K) that can be described by VRH and FAT mechanisms at low at higher temperatures respectively.

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Nitrogen and metal ions co-modified semiconductive films based on titania in ecological photocatalysis

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The growing up scientific interest to the development of the synthesis procedures directed to the creation of photocatalytically active under solar light materials can be achieved by the comprehensive approaches. The modification of semiconductor's electronic structure providing the absorption of lower energy light as well as the effective separations/trapping of photogenerated charges, the formation of appropriate surface composition and morphology for adsorption of the pollutants' species, the low-cost, fast and technologically available synthesis procedure as well as the stable, nontoxic and eco-friendly photocatalysts are required.

Herein, the correlation of the photocatalytic activity of nitrogen and metal ions co-doped titania films in the processes of environmental pollutants' degradation (tetracycline hydrochloride and dichromate ions) and their physicochemical properties is presented. Two methods of different synthesis mechanisms, namely sol-gel (liquid-phase synthesis) and pulse laser deposition (gas-phase synthesis) routes, have been used for the films' preparation. The extensive analysis of the experimental results allowed to determine the optimal synthesis conditions as well as the limitations that have to be taken into consideration. It is shown that the nature of co-doped metal ions affects the chemical state of nitrogen and its content in the film structure leading to the different photocatalytic behavior. The formation of multicomponent bonds affected the position of semiconductor energy levels and recognized as the surface active sites, are strictly determined by synthesis conditions. Some aspects of nitrogen incorporation mechanisms of sol-gel and pulsed laser deposition films' synthesis are discussed.

Clay-sulfur composition against oidium on grapes

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The clay-sulfur composition was obtained by a nanotechnological method. X-ray diffractometric and IR spectroscopic analysis of the composition showed the invariability of the structural layers of the clay, which is due to the penetration of sulfur molecules into the nanoscale structural layers of bentonite clay.

In the proposed clay-sulfur composition, against grape disease "oidium" (powdery mildew), the content of pure sulfur is 20-30 % and the content of clay is 70-80 % (by weight).

Laboratory and field tests have shown that the effectiveness of the clay-sulfur composition and pure sulfur against disease is at the same level, although the sulfur content in the composition is 2-3 times less.

Both highly dispersible powders and aqueous suspensions made from clay-sulfur compositions have been tested against powdery mildew of grape.

Finely dispersed clay-sulfur powder is sprayed faster and better than pure sulfur powder. Unlike pure sulfur powder, highly dispersed powder of clay-sulfur composition does not irritate mucous of eyes.

The powder, which is made from clay-sulfur composition, is used for the preparation of aqueous suspensions. Water is supplied in the powder, calculated amount to obtain a paste of sour cream consistency (after mixing). Further, the paste is dissolved in a certain amount of water, to obtain aqueous suspensions of the required concentrations, which are used to process the vineyards.

According to the results of a test carried out in favorable climatic conditions for the spread of powdery mildew, the development of the disease on vines treated with both pure sulfur and modifications of the clay-sulfur composition is very weak. At the same time, 70-80 % of grapes (on control vines not treated with sulfur-containing reparants) were damaged. In some cases, the intensity of the development of powdery mildew was so strong that the affected grains were completely covered with ash flakes.

Thus, using a simple and effective nanotechnological method, a clay-sulfur composition is obtained, from which a stable sulfur-containing emulsion system can be obtained, without the use of synthetic emulsifiers, which have high fungicidal and acaricidal properties.

Antimicrobial activity of the tannins isolated from walnut (*Juglans regia* L.)

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Juglans regia walnut shell is a rich source of phenolic compounds, of which the tannins manifesting high antioxidant, antibacterial and anticandidic activity [1]. The aim of the present research was to establish the antimicrobial activity of the intact and oxidized tannins isolated from the walnut septum *J. regia*.

J. regia walnut septum served as a vegetable raw material for the obtaining of the tannins. The testing of the antimicrobial activity of the tannins was performed on the bacteria *Bacillus subtilis* - gram-positive, *Pseudomonas fluorescens*, *Erwinia amylovora*, *E. carotovora*, *Xanthomonas campestris* - gram-negative, the yeast *Candida utilis*, the fungi *Fusarium alternaria*.

The extraction and oxidation of the tannins were performed by static method (maceration, periodic draining), taking into account also important factors, such as the concentration of the solvent, the ratio of plant product: solvent, extraction duration. The total content of the polyphenolic compounds was determined by spectrophotometric method with Folin-Ciocalteu color reagent [2].

The following were established: 1) intact and oxidized tannin extracts, show differentiated antibacterial and antifungal action depending on the concentration of the preparation and the species of the microorganisms; 2) the oxidation of the tannin extract led to the increase of the antibacterial activity for *E. amylovora* and *E. carotovora*, and its decrease for *B. subtilis*, the efficient concentrations being 0.15; 0.15 and 0.3 %, respectively; 3) the highest antifungal activity presented the intact and oxidized tannins in the concentration of 0.05 % for *D. sorokiniana*, followed by the oxidized tannins-0.05 % for *A. alternata* and *F. oxysporum*; 4) the tannin extracts determined the development of small spores and the inhibition of the intracellular wall biosynthesis (*D. sorokiniana*), premature germination of spores - (*A. alternata*) and an uneven development of fungal mycelium hyphae (*F. oxysporum*).

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Oak tannic compounds and their *in vitro* antimicrobial properties

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The tannins from oak bark (*Quercus cortex*) are successfully applied in the treatment of various diseases - diarrhea, stomatitis, pharyngitis and skin inflammations [1]. The aim of the research was the efficientization of the method of phenolic compounds extraction from native oak raw material, establishing their physico-chemical properties and antimicrobial activity.

Oak sawdust from wood processing enterprises from the Republic of Moldova was used as a vegetable raw material for the tannins obtaining. The testing of the antimicrobial activity of the tannins was performed on the bacteria: *Pseudomonas aeruginosa* (gram-negative), *Bacillus subtilis* (gram-positive) and the fungi *Alternaria* and *Fusarium* isolated from plants with symptoms of root rot.

To obtain the extracts from the plant material, the static method (maceration and periodic draining) and the dynamic method (ultrasonic field extraction) were used. The total content of polyphenolic compounds was determined by spectrophotometric method [2]. The total content of acidic functional groups was established based on the total content of acidic functional groups.

The bacteria *P. aeruginosa* and *B. subtilis* were grown on peptonate agar, supplemented with tannins in concentrations of 0.7...0.085 %. Screening of the antifungal activity of the tannins was performed by supplementing them in the concentrations of 0.25...0.0025 % to the PDA (Potatoes Dextrosis Agar) nutrient medium.

It was established: 1) the optimal conditions for the extracting of the polyphenolic compounds from oak sawdust are: the action of the ultrasonic field for 30 minutes at a controlled temperature, the vegetable product ratio: solvent - 1:5, the use of 50 % ethyl alcohol as a solvent; 2) isolated tannins from oak sawdust show *in vitro* antibacterial activities (*P. aeruginosa*, *B. subtilis*) in the concentrations of 0.017; 0.035 % and antifungal (*A. alternata*, *A. consortiale*, *F. oxysporum*, *F. solani*, *F. gibbosum*) in the concentrations of 0.25; 0.025; 0.0025 %, which denotes the opportunity of these compounds in the ecological protection of crop plants from various bacteriosis and mycoses.

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Absorption of *Bacillus cereus* bacteria on activated charcoal obtained from apricot husks

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The paper presents the results of scientific research related to the study of adsorption processes of bacteria within the species *Bacillus cereus* on activated carbon obtained from apricot husks in a fluidized layer. The activated carbons used have a specific BET area of about $1500 \text{ m}^2/\text{g}$ and a total sorption volume of the pores equal to $1.05 \text{ cm}^3/\text{g}$. The study of the kinetics of the adsorption processes of the bacteria within the above mentioned species showed that the value of the maximum adsorption of the bacteria is established within 2 hours.

After 2 hours of mechanical stirring, the concentration of bacteria begins to increase exponentially. After 12 hours of contact, the concentration of bacteria increases so rapidly that the bacteria coagulate forming microfuges in solution. The obtained results allow us to conclude that the bacteria in the first 2 hours are adsorbed in the macropores of the activated carbon.

After the saturation of the macropores, the activated carbon has the role of mechanical surface, which allows the rapid multiplication of bacteria. This fact is also confirmed by the research results, which are related to the study of the behavior of bacteria when stirring in aqueous solutions in the absence of activated carbon, especially the linear decrease in the concentration of bacteria depending on the contact time.

Acknowledgements

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Study of the surface chemistry modification processes of intact and chemically modified pectins and sorption of Pb(II) and Hg(II) ions on natural organic adsorbents

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The paper presents the results of scientific research that highlights the processes of pectins surface chemistry modification, obtained from apple fruits by oxidation processes. The quality and quantity of carboxylic and phenolic functional groups on intact and modified pectins were established using the Boehm method. Structural changes in the surface of oxidized pectins with hydrogen peroxide and ozone in hydrogen peroxide were determined using scanning electron microscopy (SEM) methods, FTIR spectroscopy, thermoanalytic methods TG, DTA, DTG and nitrogen adsorption-desorption.

It has been established that by oxidation with concentrated hydrogen peroxide, the amount of strongly acidic functional groups in pectin increases twice, and in the process of oxidation with ozone in concentrated hydrogen peroxide, the amount of these types of functional groups increases about three times. In the oxidation process, the polymeric chain in pectins breaks with the formation of fragments with lower molecular weights. This fact was confirmed by the SEM, FTIR methods, thermal analysis and adsorption-desorption of nitrogen applied on intact and oxidized pectins. The sorption processes of Pb(II) and Hg(II) ions on intact and chemically modified pectins were studied. It has been shown that the immobilization capacity of heavy metal ions in aqueous solutions is directly proportional to the value of strongly acidic carboxylic groups in intact and chemically modified pectins.

Acknowledgements

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Dynamics of Sr²⁺ ion adsorption from aqueous solutions on activated carbon CAN-7

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The dynamics of adsorption of strontium ions from aqueous solutions was studied on concentrated solutions of CAN-7 activated carbon, at different lengths of the adsorbent column working layer and at different solution filtration rates.

The following parameters were determined based on the breakthrough curves of strontium ions from aqueous solutions on CAN-7 activated carbon at the solution filtration rate of 10 mL/min: (i) the length of the working layer of the adsorbent column, (ii) the length of the inactive layer, (iii) the speed of movement of the adsorbent front and (iv) the travel time of the adsorbate carrying solution through the working layer of the adsorbent.

The results obtained showed that the adsorption of strontium ions depends on the diffusion coefficient of these ions in the porous structure of CAN-7 activated carbon and on the surface chemistry of the activated carbon used.

The possibility of enlarging the working layer of the activated carbon column and the possibility of reducing its inactive layer were analyzed.

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Corrosion stability and hydrogen permeability of the medium-carbon steels with surface nanocrystalline layer

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One of the known methods of formation of surface nanocrystalline structures is mechanical-pulse treatment [1] which used high-speed friction for severe plastic deformation of the surface layer. It can be realized on surface-grinding and treated-turning machines after insignificant modification. Under mechanical-pulse treatment technological environments with polymer additives and powders of alloying elements are supplied to the friction contact zone. Mechano- and thermodestruction of polymer additives [2] occurred due to high pressure and temperature in the friction contact zone. The fragmentation of the surface layer's structure to the nano sizes (10–12 nm) with its simultaneous saturation by polymer components and alloying elements took place during mechanical-pulse treatment. The dislocation density achieved 10^{12} cm^{-2} .

It has been shown that adding nickel, boron and nitrogen-containing substances into technological environment during mechanical-pulse treatment of the 35 and 45 carbon steels leads to alloying the surface layer with these elements and, consequently, to increasing their resistance to corrosion. Such treatment can offset the negative influence of intensive plastic deformation on corrosion resistance of carbon steels.

It has been found that the nanocrystalline surface layer serves as a barrier for hydrogen penetration into the bulk material. The surface layer with nanocrystalline structure formed on the 45 steel by mechanical-pulse treatment is characterized by lower hydrogen permeability (hydrogen diffusion coefficient is in 1.3–4 times lower) and higher in 1.5–4.4 times efficiency of hydrogen trapping in comparison with the untreated steel. Therefore, it serves as a barrier for hydrogen penetration into the bulk material.

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SEM-EDX study of compressed aluminum powders mechanochemically activated by low-melting alloys and graphite

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Activated aluminum is a promising material for producing hydrogen by its hydrolysis. In the present work, the mechanochemical activation of PA-4 (particle sizes < 100 µm) and ASD-1 (particle sizes <30 µm) aluminum powders by Ga-In-Sn or Ga-In-Sn-Zn eutectic alloys (5 wt.%) and by graphite (3 wt.%) was carried out in a mixer ball mill SpexCerti Prep 8000-D during 1, 2 or 4 h in an argon atmosphere. The activated Al powders were compressed ($P = 4$ MPa) into pellets ($\varnothing = 1$ cm, $m_{\text{pellet}} = 0.2$ or 0.3 g) under argon. The morphology and composition of the pellet surface were studied using a Zeiss EVO 40XVP scanning electron microscope with an INCA Energy microanalysis system.

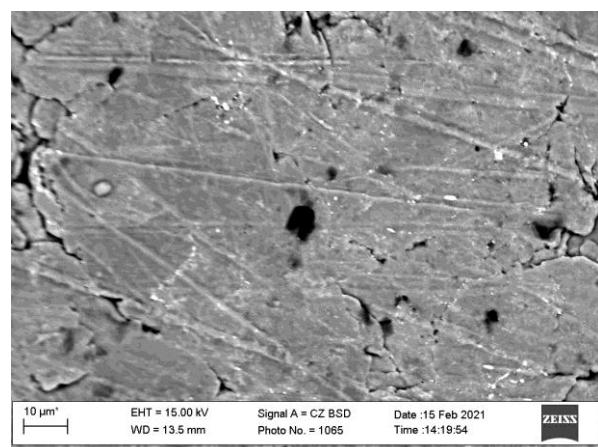
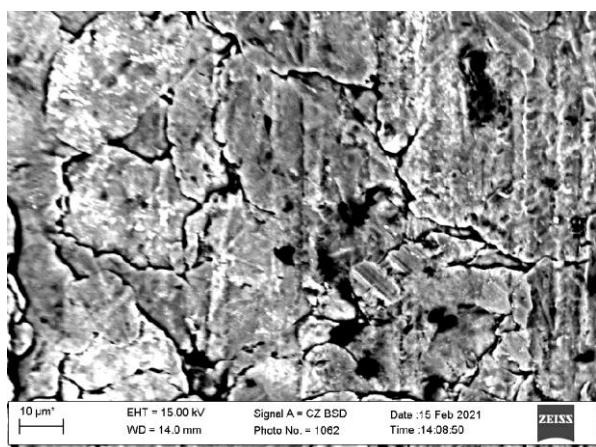


Fig. 1. SEM micrograph of the surface of pellet made from ASD-1 powder activated by Ga-In-Sn eutectic alloy (5 wt.%) and graphite (3 wt.%)

Fig. 2. SEM micrograph of the surface of pellet made from PA-4 powder activated by Ga-In-Sn-Zn eutectic alloy (5 wt.%) and graphite (3 wt.%)

As follows from the Figs. 1 and 2, there were interfaces between grains of the activated and compressed aluminum powders, on which activating elements were located. The average quantitative composition (wt.%) of the pellet surface was as follows: Al – 94.64, Ga – 3.13, In – 1.33, Sn – 0.90 (Fig. 1) and Al – 93.41, Ga – 3.67, In – 1.78, Sn – 1.14 (Fig. 2). The components of activating eutectic alloys were very uniformly distributed over the surface of the pellets. The graphite, on the contrary, was mainly situated locally; its content in the places of dark spots in Figs. 1 and 2 was about 75 wt.%.

Interaction of cationic dyes with DNA sorbed onto nanocrystalline dioxide titanium and ceria surfaces

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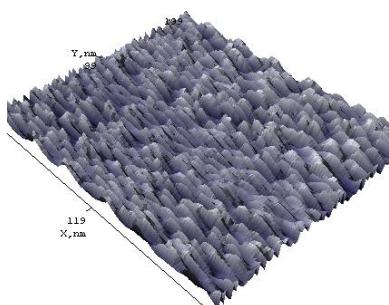
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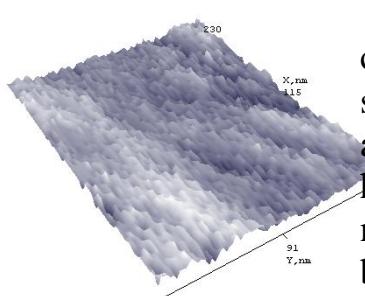
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The nanosized materials are widely used in biotechnology, medicine, environmental chemistry due to their biocompatibility, physicochemical stability lack of toxic effects. At the same time the DNA molecule is the main object of nanothechnology as reservoir for local drug delivery or instrument for the treatment of genetic diseases by searching for potential intercalators. The combination of nanooxides and DNA molecules can lead to the creation of new materials which could be as antitumor, antibacterial, and antiviral agents to block the disease pathway at an early stage. The planar heterocyclic molecules, including natural and synthetic dyes, are known to interact with nucleic acids. This property is successfully used for medical, analytical purposes and for diagnosis. The question arises whether the DNA molecule attached to the surface of solid remains capable of interacting with intercalators.

The adsorption of proflavine and methylene blue at oxides and oxide/DNA surfaces was studied. It was shown that the preliminary adsorption of DNA onto TiO₂ (or CeO₂) surface does not interfere with the fact and way of its interaction with dyes, which is confirmed by diffuse reflectance spectroscopy and atomic force and scanning electronic microscopy methods. It is noted that proflavine, intercalating into DNA molecules, promotes the formation of larger elongated fragments with clear boundaries between them, forming an ordered anisotropic relief (AFM-image 1). Whereas methylene blue forms a more uniform relief, interacting with DNA, as if covering the sample surface by a layer of molecules (AFM-image 2).



AFM-image 1. TiO₂-DNA-
Proflavine



AFM-image 2. TiO₂-DNA-
Methylene blue

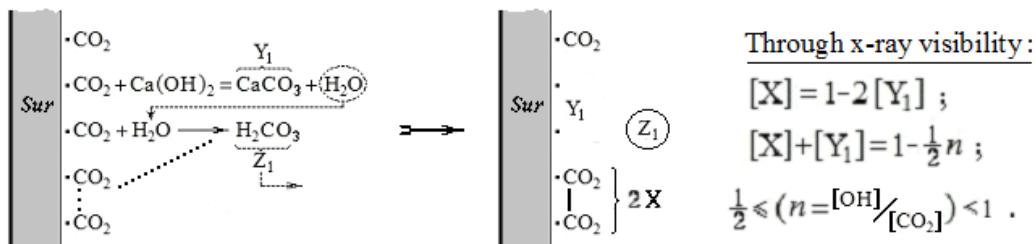
These composites can serve as model structures for research and development of new hybrid materials in the nanobiotechnological and biochemical fields.

Cooperative emergence of vaterite and graphene oxide nanoclusters in the calcium-surfactant-nanocarbonate interfaces

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The studying of the lipophilic carbonate nanomicelles started with the development of manufacture of dispersive-detergent additives to motor oils and, moreover, the overbased calcium greases [1]. Thixotropic calcium carbonate systems with nanomicelle of 7 to 30 nm are synthesized by a carbonation of reciprocal emulsions for calcium-hydroxide water-methanol solutions dispersed in oil-toluene phase with surfactants. Their orientations cause the carbonate growth in preferred directions and self-organization of CO₂ conversion on a quantum level. For synthesis with CO₂ gas, the results of XRD and electrophysical investigations for calcium-sulfonate (alkylsalicylate, phenolate, carboxylate)-nanocarbonate are indicated a high probability of different carbonaceous processes with electrostatic "emersion" of the intra-micelle GO clusters [2], that has found evidence from our experiments:



Reverse correlation with a factor of 2 between the [X] and [Y₁] concentrations is a unique to identify and study of the crystalline structure of X nanophase. For as-prepared nanoheterogeneous calcium carbonate systems with various surfactants, the Y₁ nanophase has a structure of vaterite, whereas the X nanophase is graphene-derived which may has CO₂ stoichiometry. For some comparison there are the results of [3]. Numerical evaluations of XRD results contribute to the assumption that vaterite nanophase (Y₁) within depot (Sur) is framed in the form of parallel nanoplanes that is possible in nature [4]. Accordingly to Scherrer estimation the characteristic size of carbonic nanophase (X) is 4-5 nm, that is 13-15 of its interplanar distances.

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Influence of interaction of the polymer component in polymer blend on their melting temperature

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Polymer composites are widely used as structural materials in high technology industries, since their properties can be easily changed for a specific task.

There were produced two-component systems on the base of polypropylene (PP-Fe) and copolyamide (CPA-Fe) filled with dispersed iron. Three-component system PP/CPA-Fe also was prepared, wherein the CPA-Fe increases from 0 to 100 %, the Fe content rises from 0 to 40 vol.%, accordingly, the PP component is changed from 100 to 0 %. The values of melting temperature (T_m) for PP-Fe and CPA-Fe composites (Fig. a), that were obtained from TMA measurements, have a minor increase in a whole range of filler concentration.

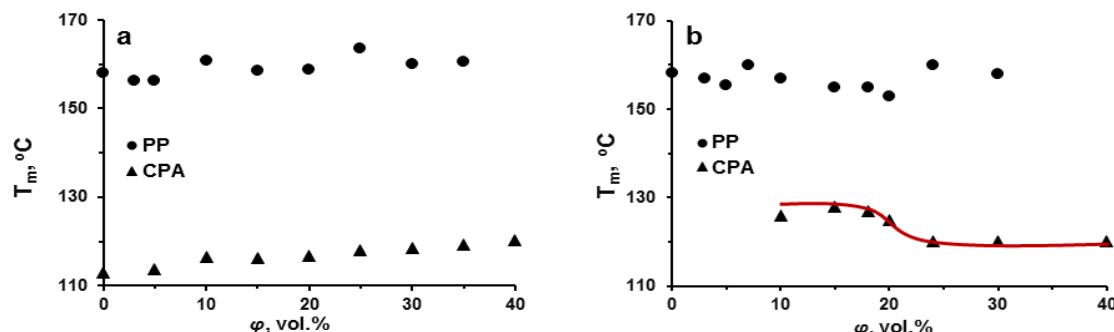


Fig. Concentration dependence of melting temperature of polymer phase in PP-Fe, CPA-Fe (a), and PP/CPA-Fe (b) composites

In the PP/CPA-Fe polymer blend the T_m value of CPA in the concentration range 24-40 vol.% of Fe remains constant. However, with decreasing Fe content, the melting point of CPA begins to increase (Fig. b). This is because of when the CPA phase melts, the PP phase is still in a solid-state, which leads to the appearance of excess pressure in the melted CPA phase. From the literature, it is known that with increasing pressure (P) on the polymer, its melting point increases, and for many polymers, the ratio $\Delta T_m / \Delta P$ is approximately equal 0.18 K/MPa. The calculation for 75PP/15CPA-10Fe composite gives the value of excess pressure $P \approx 45$ MPa. Thus, interaction of the polymer components in polymer blend leads to a shift in the melting temperature of the low melting component (CPA) to higher temperatures.

Silicene layers as a molecular container for anti-aromatic systems

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The initial model was a double-layer silicene consisting mostly of 64 silicium atoms. The lattice structure is described in parameters Si(111) - ($\sqrt{3} \times \sqrt{3}$). The plane distance is 0.511 nm. Cyclobutadiene molecules are placed into the interplane space (Fig.).

The basic structure has been optimized by the MM+ method. At the subsequent calculation stage we have applied the semi-empirical PM3 method. For further modeling, we have used the Monte-Carlo algorithm, within the temperature range 0-500 K. There have been calculated the UV-spectra of the complexes. The modified Benes-Hilderbrand method enabled to find the association constant of the “silicene / cyclobutadiene” system.

The calculations made demonstrate the potential capability of cyclobutadiene’s physical sorption in the interplanar space of double silicene layer. The crystalline grid does not have considerable structural changes, what allows to stabilize and keep unstable molecules not only at low temperatures but also at ordinary ones.

The program varied the cyclobutadiene ratio from 4 to 1 at constant concentration of double-layer silicene. Optical density was calculated at 198 nm, which is recommended in the reference literature for complexes with silicene.

In the calculation spectra we have observed a hypsochromic shift. With such component ratio it is theoretically possible to create complexes of types 1:1 and 1:2. However, the results of spectra processing by the Benes-Hilderbrand method favour the structure of type 1:1, and the stability constant of this complex is $118 \text{ l} \cdot \text{mol}^{-1}$ with the calculation accuracy $r \geq 0.99$.

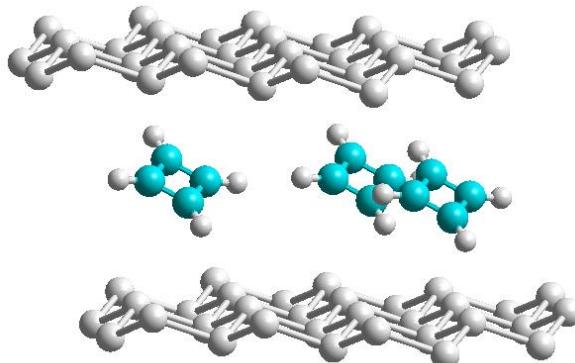


Fig. Double silicene layers containing three cyclobutadiene molecules ($T = 300 \text{ K}$)

Synthesis of polymer hybrid composites based on epoxide oligomer in the presence of nano-sized functional fillers

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The development of modern technology and industry is inextricably linked to the creation of new polymeric materials, among which the hybrid organo-inorganic composite polymeric nanomaterials are becoming important. The great interest is explained by the possibility of creating systems with a wide range of properties that can be adjusted allowing to receive the materials with the specific characteristics for multi-purpose use.

The aim of this work was to study the process of the structure formation as well as the physical and mechanical characteristics of polymer hybrid compositions based on epoxy oligomer and inorganic nanosized filler - aerosil with different surface nature.

The objects of research are the hybrid organo-inorganic polymer nanocomposites based on epoxydian oligomer brand ED-20 and inorganic component in the form of the powdered nanosized inorganic silicon dioxide (SiO_2) - aerosil. Aerosil brand A-300 with unmodified surface and aerosil brand AM-300 with industrially hydrophobized dimethyldichlorosilane surface were used in the work. The content of nanofiller in the composite was from 0.1 to 15 %.

The results obtained by thermogravimetry showed that the introduction of highly dispersed aerosil A-300 and modified AM-300 in the amount of 0.5 % in the epoxy matrix did not lead to a significant change in the thermal properties of the studied nanocomposites.

The obtained data of radiographic studies and the results of the physical and mechanical tests showed that in the formation of the two-level nature of the nanofiller structure tensile strength of epoxy nanocomposites was extremely dependent, when filling the composite with aerosil about 0.5 %, which may be a consequence of the formation at such concentrations of a continuous reinforcing mesh, which is formed by adjacent mass-fractal aggregates.

It was established that the presence of active groups on the surface of the inorganic phase, which can react with the epoxy matrix, affected the morphology of the composite and its properties.

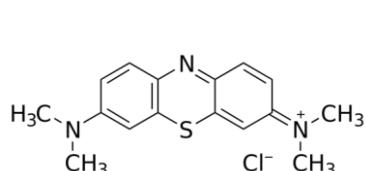
Hydrogels based on the graft copolymers of chitosan and their sorption-desorption properties

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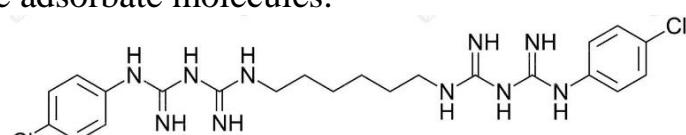
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Hydrogels based on copolymers of chitosan possess unique properties such as non-poisonous, biocompatibility, biodegradability and non-carcinogenic [1]. Therefore, chitosan has potential utilities in various fields like biomedicine, as antimicrobial agent, wastewater treatment, food packaging functional membranes and flocculation. Cross-linked copolymers Chitosan-graft-Polyacrylamide (Ch-g-PAA) were prepared by using N,N'-methylene-bis-acrylamide as cross-linker during radical polymerization of two component system. In this work, redox initiator such as CAN (ceric ammonium nitrate) was used to initiate graft copolymerization. FT-IR, TGA and DSC studies of hybrid polyacryamide hydrogels were carried out to analyse its structure.

Sorption/desorption properties of hydrogels in relation to the biologically active chlorhexidine and methylene blue were studied. These compounds may be used both to disinfect the skin of the patient and the hands of the healthcare providers. Released concentration and desorption rate of chlorhexidine and methylene blue were investigated as an important factors for regulation of therapeutic concentrations of the active substances in bacteria medium. It was found the greater chitosan content in hydrogels the slower desorption process and lower released concentration of the adsorbate molecules.



Methylene blue



Chlorhexidine

Chemical structures of the adsorbate molecules

The obtained results permit the conclusion that grafted chitosan has the potential to be used wound-healing management and targeting drug release studies. The great sorption capabilities of grafted chitosan for dye molecules can be of great use for wastewater treatment and the recovery of metals and also the treatment of polluted effluents.

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Adsorption of Co(II) and Sr(II) ions from aqueous solutions onto oxidized vegetal activated carbons

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The presence of heavy metals in the environment is a major concern due to their toxicity to many life forms [1]. The adsorption process is one of the water treatment techniques which is used to remove the toxic metal ions [2,3].

Activated carbons of local origin (Republic of Moldova) from the apple wood (CA-M) and nut shells (CA-N) were oxidized with nitric acid (sample CA-M_{ox}) and mixture of nitric acid/urea (samples CA-M_{ox-u} and CA-N_{ox-u}) in order to improve their ion-exchange properties. The morphological, textural and surface properties of the activated carbons were analysed by using standard techniques, such as: SEM-EDX; N₂ sorption-desorption isotherms for determination of surface area (S_{BET}) and micropore volume (V_{micro}); the surface functional groups were quantified by Boehm titration method and FTIR analysis. Obtained results showed that after oxidation process the surface area and total pore volume of oxidized samples is reduced by about 15%; at the same time, carboxylic, aldehydic and ketonic groups are formed on the carbon surface. Bath-mode adsorption experiments were carried out to remove Co(II) and Sr(II) ions from aqueous solutions. Equilibrium adsorption data of metal ions on activated carbons were fitted by using four isotherm models: Langmuir, Freundlich, Temkin and Dubinin-Radushkevich. In order to analyze the obtained kinetic data three kinetic models: pseudo-first order model, pseudo-second order model, and intraparticle diffusion model were used. The adsorption equilibrium data obeyed the Langmuir and Dubinin-Radushkevich isotherms. The kinetics of the adsorption of Co(II) and Sr(II) ions followed the pseudo-second-order equation. According to the obtained data, the best sample for adsorption of Co(II) and Sr(II) ions is CA-M_{ox}, with an adsorption capacity of 0.075 and 0.096 mmol/g, respectively.

Acknowledgements. This work was partially supported by State Program (2020-2023) Project "Reducing the effects of toxic chemicals on the environment and health through the use of adsorbents and catalysts obtained from local raw materials" (ANCD/20.80009.7007.21) and Horizon 2020 Programme MSCA-RISE-2016, Project NanoMed No. 734641.

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Influence of different types of pretreatment on catalytic pyrolysis of model lignin compounds

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Recently, more and more attention has been paid to the use of lignin as a natural renewable raw material for the production of chemicals. Catalytic depolymerization of lignin and subsequent upgrading of the resulting products using catalytic pyrolysis can provide access to biofuels and a wide range of chemicals. The development of new methodological approaches to catalytic pyrolysis makes it possible to control both the qualitative and quantitative composition of the final products. The aim of our work was to study the effect of different methods of pretreatment on the pyrolysis kinetics of model lignin compounds over nanoceria catalyst.

4-Methoxycinnamic, coumaric and cinnamic acids served as model lignin compounds. The structure of complexes of the model lignin compounds on the nanoceria surface was studied using FT-IR spectroscopy. Their thermal transformations were investigated using the temperature-programmed desorption mass spectrometry method using a MKH-7304A monopole mass spectrometer (Sumy, Ukraine) with electron impact ionization adapted for thermodesorption measurements. The obtained IR-spectroscopic data indicate the interaction of the carboxyl groups of the studied acids, as well as the methoxy and hydroxy functional groups with the nanoceria surface. For the studied acids, the presence on the nanoceria surface of carboxylate complexes with bidentate bridging and bidentate chelate structures was revealed. The main processes occurring during the catalytic pyrolysis of acids were decarboxylation, decarbonylation, and dehydration.

Acknowledgements

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The TEM images-based predictive modeling for differently shaped Rh nanoparticles classification in a hybrid photocatalyst

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On the basis of our article [1], data analysis of the size distribution profiles for three differently shaped Rh-modified TiO₂ subject samples, NP (spherical), NC (cubic) and Oh (octahedral), was performed with the help of the following techniques: distributions classification, analysis of variances, discriminant analysis. The materials feature in Rh nanoparticles' morphology-dependent photocatalytic activity. The results allowed us to distinguish the types of the samples by their particles size distribution profiles and develop the models to classify them. The proposed algorithms can be deployed for identification of each sample from TEM images. To this end, machine learning approaches, such as non-parametric K-Nearest Neighbors ($K_{max} = 100$, metrics: Euclidean distances at the uniform weight of each point), Naïve Bayes, Logistic Regression, Bootstrap Forest (1 split per sample, learning rate 0.1, 35 trees) and Classification Tree (9 splits) were trained, validated and their effectiveness to predict the samples (output) by their size distribution profiles (input) was compared. The most precise model has turned out to be Logistic Regression, whose misclassification rate (MR) at the validation stage is less than 8 % (7.64 %). This model's other metrics, Generalized R² and Entropy R², are the highest among the models at the same MR, such as Naïve Bayes and Bootstrap Forest (Fig.). As a result, an offline HTML-calculator for Logistic Regression was developed and provided on [https://github.com/Nazarkovsky/Rh-TiO₂-classifier](https://github.com/Nazarkovsky/Rh-TiO2-classifier) to predict the samples type. The project was coded by means of JSL (SAS) [2].

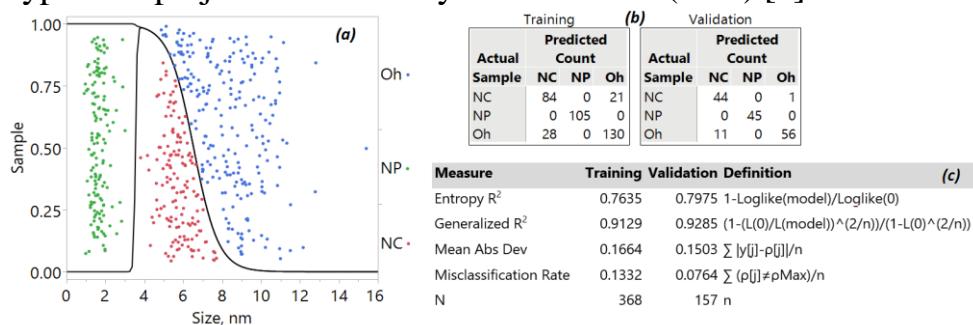


Fig. Logistic plot (a), confusion matrices for training and validation (b), and the model's measures (c)

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Adsorption modifying of nanosilica with lignin in a gaseous dispersion medium

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The aim of this work was to test the applicability of the gas-phase methods of modifying developed in Chuiko Institute of Surface Chemistry of NASU for adsorption modifying of nanosilica (fumed silica, $S_{BET}=300 \text{ m}^2/\text{g}$, Ukraine) with a complex three-dimensional network polymer having an aromatic nature – lignin (Lignosulphonate DP-1962, Norway).

Adsorption interaction with organic molecules that have polar functional groups occurs as a result of the formation of hydrogen bonds with silanol groups. The degree of perturbation of the $\equiv\text{Si}-\text{OH}$ groups characterizes the degree of surface coverage (Θ). The IR spectra of modified silicas and the indicated dependences are shown on Fig. Previously, we found for linear macromolecules of POE and PVP that when the polymer content on the surface of nanosilica is $\sim 200 \text{ mg/g}$, all silanol groups are perturbed. As can be seen from Fig. b, in this case, the degree of perturbation was $\sim 40 \%$. We believe that this is due to the three-dimensional structure of the lignin molecule. Thus, this method allows to create a cover from lignin on the nanosilica surface.

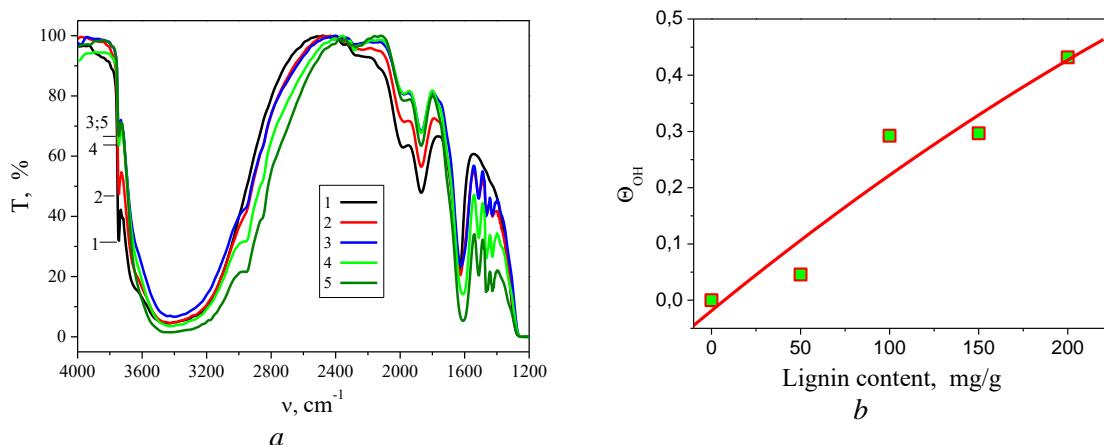


Fig. IR spectra of nanosilica: 1 - initial, 2-5 - containing 50, 100, 150 and 200 mg/g of lignin, respectively (a). Dependence of the degree of perturbation of surface silanol groups of nanosilica on the lignin content (b)

Acknowledgements

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The effect of the izoelectric point values of the gelatin on its adsorption onto nanosilica surface at various pH

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Gelatin adsorption on the surface of nanosilica was studied at pH range from 3 to 8. Three types of gelatin were used in the study: *a*) edible gelatin with an isoelectric point (pI) value of 4.3–4.8; *b*) from the Merck catalog (pI = 4.3–4.8) and *c*) from the Fluka catalog (pI = 7.5-7.7) (Fig.1).

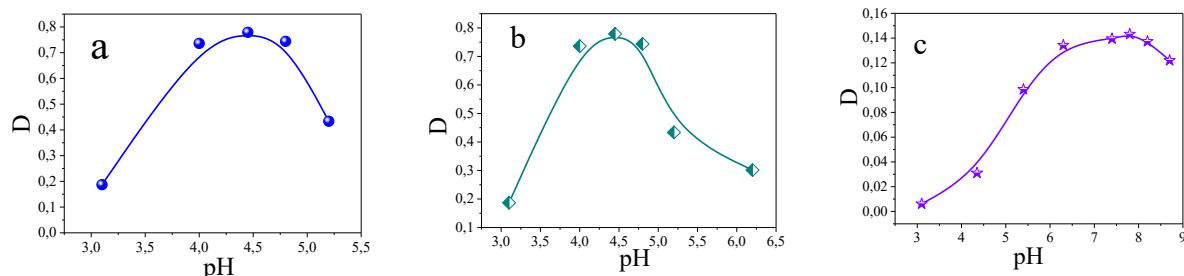


Fig. 1. Dependences of the optical density D ($\lambda = 800$ nm) of gelatin solutions at various pH for the gelatin *a*, gelatin *b*, gelatin *c*

It has been shown that for gelatin *a* and *b*, the adsorption curves have a maximum at $\text{pH} \sim 4.5$ -5; and for gelatin *c*, the adsorption monotonically increases with increasing pH (Fig. 2).

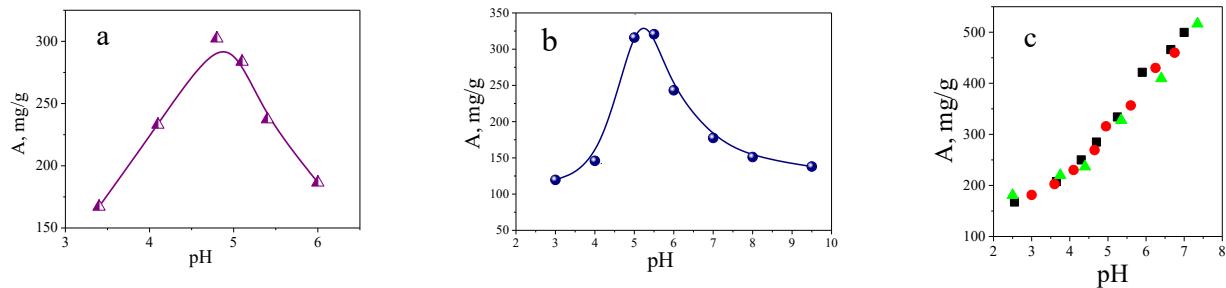


Fig. 2. Dependences of the gelatin adsorption on the nanosilica surface at various pH for the gelatin *a*, gelatin *b*, gelatin *c*

It was noted that at $\text{pH} \sim 5$, the adsorption values for the three types of gelatin (gelatin *a*, gelatin *b*, gelatin *c*) were approximately equal.

A comparison was carried out of the adsorption activity of nanosilica relatively to proteins determined from isotherms and of that found by the method of point measurements. It has been found that the adsorption value of gelatin *a* onto the nanosilica at $C_{\text{initial}} = 700$ mg/100 ml is equal to the A_{ave} value determined by the Langmuir isotherms. This fact verifies the applicability of the method of point measurements for nanosilica/gelatin system to characterize the pharmacological activity of nanosilica based enterosorbents.

Optimization of technological parameters of nanocomposites of the multiwalled carbon nanotubes and polyvinyl chloride, polyethylene, porous polystyrene

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The influencing of ultrasonic deformation ϵ_{US} was researched on anelastic and elastic characteristics of nanocomposites of multiwalled carbon nanotubes (MWCNT). The quasitransversal ultrasonic (US) velocity $V_{\perp} = 768 \pm 30$ m/sec, shear module $G = \rho V_{\perp}^2 = 578$ MPa, the quasilongitudinal US velocity $V_{\parallel} = 2485 \pm 30$ m/sec, dynamical elastic module $E = \rho V_{\parallel}^2 = 6.057$ GPa, Poisson coefficient $\mu = 0.442$ specific density polyethylene with low density high pressure $(C_2H_4)_n + 3\%$ MWCNT were determined from the oscilloscopegramma [1] in Fig.

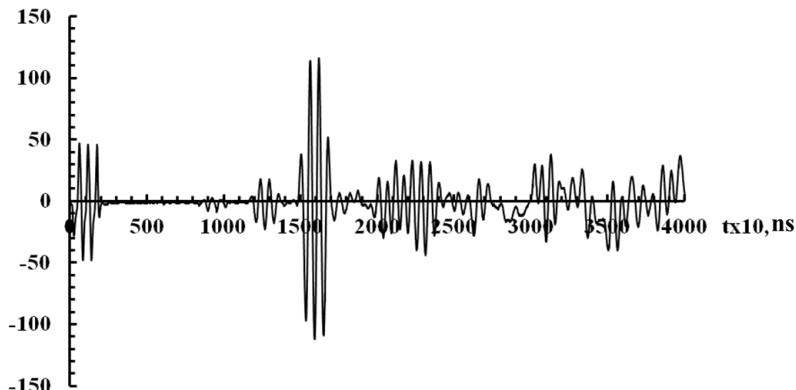


Fig. The oscilloscopegramma of quasitransversal elastic waves velocity measuring $V_{\perp} = 768$ m/sec in nanocomposite polyethylene with low density high pressure $(C_2H_4)_n + 3\%$ multiwalled carbon nanotubes by impulse-phase method at frequency $f_{\perp} = 0.7$ MGz

Conclusions

1. The increase of the nanocomposite crystalline degree at growth of multiwalled carbon nanotubes concentration filling with the nanotubes of matrix results in the decline of content of well-organized phase.
2. The annealing of the structure defects in nanocomposites bends out of shape the type of internal friction temperature spectrum $Q^{-1}(T)$.

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On microstructure of nanosized iron oxide (magnetite)

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In this work, the results of studying the microstructure of nanoscale iron oxide using structural analysis methods are presented. Iron oxide Fe_3O_4 (magnetite) synthesized by co-deposition of iron salts stabilized by oleic acid, was selected as an object of research. The XRD and TEM/(HRTE methods have been used. The crystallite size distribution (CSD) based on full profile diffractogram analysis by WPPM [1] and regularization [2] methods and the TEM particle size distribution (PSD) were constructed. The average size of iron oxide crystallites was also estimated using the Scherrer equation. The microstructure parameters obtained from X-ray data were compared with electron microscopy images (Fig.).

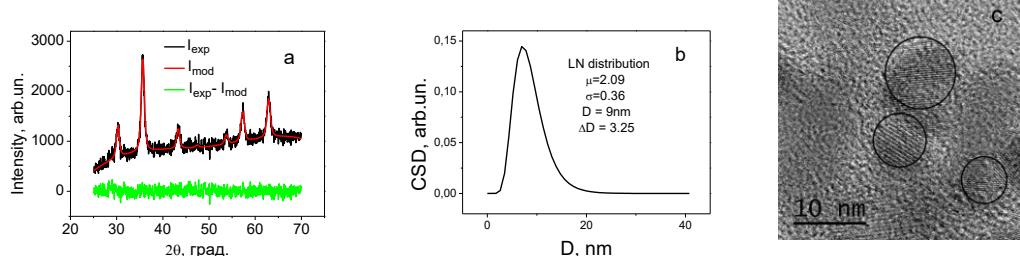


Fig. Results of XRD (a), WPPM (b), HRTEM (c) analysis of nanosized Fe_3O_4

The data of all methods confirm that the sizes of crystallites and particles of magnetite have comparable in magnitude values. They average 9-11 nm. Using the WPP method, assuming the lognormal distribution of spherical crystallites, the smallest value of the average crystallite size is determined. The regularization method used for the profile analysis of (311) diffraction peak of Fe_3O_4 showed the best agreement between the CSD and PSD by TEM and consistency with the estimation of the average size of crystallites by Scherrer [3].

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Phase composition and magnetic properties of nanopowders obtained by processing of Mn(Fe, Co)/Bi/La nitrates mixtures under hydrothermal conditions

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Development of promising methods for the synthesis of composites based on metals/metals oxides with adjustable magnetic properties is one of the most important tasks in the chemistry of nanomaterials [1, 2].

The report presents the results of studies of the phase composition and magnetic properties of products of hydrothermal treatment at a temperature of 200 °C for 3 hours in an autoclave of a mixture of Mn (Fe, Co), Bi and La nitrates, taken in a ratio of 1:2:1 in ethylene glycol and formic acid. The synthesized oxide composites have been characterized by X-ray diffractometry, IR and EMR spectroscopy. The EMR spectra of the some synthesized composites are presented in Fig.

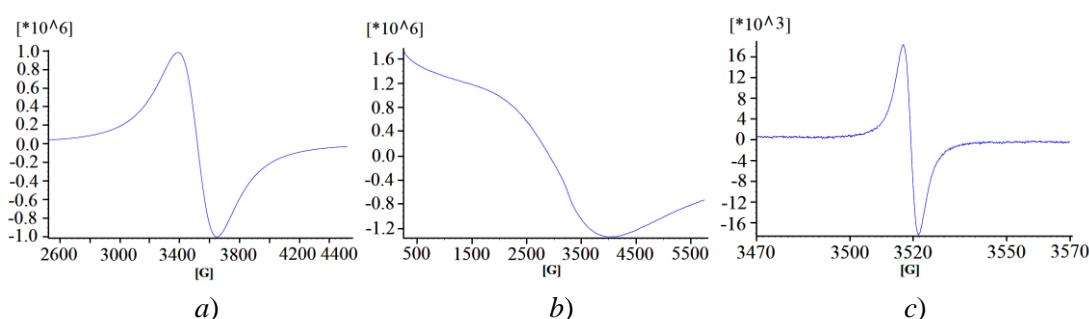


Fig. EMR spectra, recorded at room temperature, of: a) Mn/Bi/La; b) Co/Bi/La, c) Co/Bi/La (1:2:1) synthesized in formic acid (a, b) and ethylene-glycol (c) medium

The influence of the medium on the phase composition and magnetic properties of the synthesized composites is discussed.

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Acid-base properties of catalysts based on aluminosilicate for hydrogenation of carbon dioxide according to EPR spectroscopy of adsorbed nitroxyl radicals and thermal desorption of adsorbed methanol

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Carbon dioxide is the main source of the greenhouse effect that causes global warming and climate change. At present CO₂ is considered as an alternative to fossil fuels as a source for processing into chemical products, including methanol, which is a key raw material for the chemical industry. Hydrogenation of CO₂ to methanol is the one of the most attractive way to convert CO₂ [1, 2]. In this report the results of studies of the acid-base peculiarities of Co, Pd-containing catalysts based on SIRAL aluminosilicates produced by "Sasol" with the composition SiO₂/Al₂O₃ = 1; 10; 40 by EPR spectroscopy of adsorbed nitroxyl radicals (NR) and thermal analysis in the mode of thermoproduced desorption of methanol. Figure shows the structure of the used NRs.

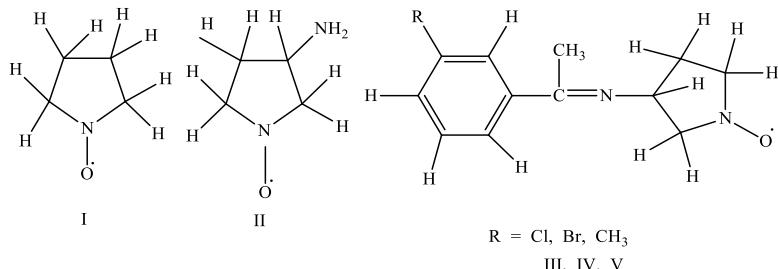


Fig. The structure of the used NRs

Before measurements, the catalyst samples were calcined at 500 °C for 6 hours, then treated in a nitrogen flow for 30 min, cooled to room temperature, and saturated with methanol vapor. Nitroxyl radicals were adsorbed from organic solutions. Thermal analysis of the samples with adsorbed methanol was carried out using "STA-449 F3", NETZSCH analyzer in a stream of gaseous nitrogen at a temperature rise rate of 10 °/min. EPR measurements were performed using a Jeol JES-PE 3XQ spectrometer.

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Synthesis and composition of some copper(I) maleates

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The elemental composition and features of the morphology of the copper-organic dispersion with maleic acid (MA) as an organic component have been determined by the method of energy-dispersive X-ray spectroscopy [1]. The organo-copper dispersion by precipitation copper with zinc dust has been obtained. Energy-dispersion analysis has been performed for copper, carbon and oxygen atoms. Hydrogen atoms were not determined in this method of analysis. The results of the elemental analysis are shown in Table. Thus, the empirical formula of CuC_4O_6 has been established. In this case, according to thermogravimetry, it is confirmed that this dispersion in its composition included water molecules. The synthesis was carried out in a strongly acidic solution at $\text{pH} \approx 1$. At this pH, Cu^+ -ions can form relatively stable π -complexes with molecular and dissociated in the first degree forms of MA [2]. Furthermore, the complexes $[\text{Cu}^+(\text{C}_4\text{O}_4\text{H}_4)]_{\text{Aq}}$ and $[\text{Cu}^+(\text{C}_4\text{O}_4\text{H}_3)]_{\text{Aq}}$ in a solution of this pH are in the same amount. With the using of quantum chemical modeling, the features of geometric and electronic structure for complexes of similar composition have been analyzed in detail [3]. If we compare the results of the elemental analysis of the selected fragment of powder (Table) with possible model forms of complexes of copper(I) with MA, then we get a fairly close coincidence with the structures $[\text{Cu}^0(\text{C}_4\text{O}_4\text{H}_4)(\text{H}_2\text{O})_2]$, $[\text{Cu}^+(\text{C}_4\text{O}_4\text{H}_4)(\text{H}_2\text{O})_2]$ or $[\text{Cu}^+(\text{C}_4\text{O}_4\text{H}_3)(\text{H}_2\text{O})_2]$, which contain 23.1 at.% C, 46.2 at.% O, 30.8 at.% Cu.

Table. Results of elemental analysis of organo-copper powders obtained by a chemical method in the presence of maleic acid

Element	Composition, mass%	Composition, atomic%	Definition error, %
C	9.35	22.83	10.58
O	25.76	47.22	6.60
Cu	64.90	29.96	3.84

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Formation of solid compositions with mineral filling having a cleansing effect

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The use of composite materials with bioactive substances (BAS) with controlled release allows us to obtain various forms of agents - from dilute suspensions up to solids, entering towards the liquid phase immediately before use. This allows resolving the problem, arising with different shelf-life of individual components in multicomponent tools.

In this paper, the preparation routes of composites with clay minerals, diatomaceous earth and highly disperse silica-based are analyzed. In the composites, various forms of active substance are provided due to the structural hierarchy of solids used, composition optimization, and improvement of the formation techniques. Significant hydrophilicity of clays increases wettability of the materials that results in possible enhancement of BAS content in the composites.

On the basis of clays, diatomaceous earth, and plant components, the composite materials (clay/diatomaceous earth and clay/vegetable raw materials/diatomaceous earth) were prepared using mechanochemical activation. In order to assess the level of safety of the prepared composite materials, the software product "Rana" was used. This information system was designed to store and systematize the composition and calculation of the development of cosmetics and other products or fillers, determining their level of safety in terms of component composition of the final blend. The safety level assessment is based on three indicators such as Cancer, Developmental & Reproductive Toxicity, Allergies & Immunotoxicity. The indication is given in colors: Green - from 1 to 33 (appropriate level), yellow - from 34 to 77 (with some problems), and red - from 78 to 100 (negative results).

Thus, optimal composite materials were developed using clay/vegetable raw materials/diatomite. The indicators were used to evaluate the level of safety of components and composite materials and the possibility of their use in cosmetics since the hypo-allergenicity of the studied systems is confirmed. Kinetic studies of BAS release can be used to regulate the preventive action of composite shampoos.

Textile nanocomposite filters for efficient removal of organic dyes from water

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In the present work, a polymer composition based on acrylic polymer, cross-linked agent and ZnO nanoparticles was used to functionalize the polyester fabric by two routes: one bath pad method and blade coating method. The possibility of applying such fabrics as filters was explored for polluted water with cationic - methylene blue (MB) and anionic - methyl orange (MO) organic dyes.

It was established that the surface area of the fabric filter greatly dependent upon the way of treatment of polyester surface: 5.9 m²/g (polyester), 85.2 m²/g (padded polyester), 44.6 m²/g (covered polyester). Untreated polyester exhibited poor hydrophobicity with a water contact angle (WCA) of 30.6° and poor water resistance. The padded polyester demonstrated a WCA of 60.8°, and the covered one had good hydrophobic properties with a WCA of 100°. The developed filters were tested to purify water from organic dyes ($V = 25$ ml, composite layer = 0.59 g, $t = 120$ sec, filter area $S = 56$ cm²). It was shown, that the concentration of MB decreased from 100 to 60 ppm using the padded polyester, and the content of MO declined from 100 to 40 ppm assisting the covered polyester (Fig.). These observations indicate that organic dyes of different nature can be effectively removed from the water by using of suitably processed textile filter.

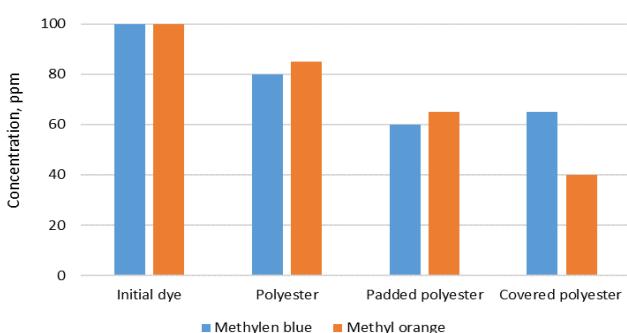


Fig. Comparison of filtration efficiency of polyester-based filters to organic dyes

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Removal of U(VI) compounds from aqueous solutions using inorganic composites based on amorphous TiO₂ modified with cobalt hexacyanoferrate(II)

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Earlier the authors have developed polymer-inorganic composites based on ion exchange resins for sorption of U(VI)-containing cations [1] and anions [2] from aqueous solutions. Fibrous polymer ion-exchangers were also tested [3], inorganic sorbents based on hydrated zirconium dioxide and zirconium hydrophosphate containing graphene-like material were synthesized [4]. The sufficient advantage of inorganic sorbents over polymers is stability against ionizing radiation.

Here the composites based on hydrated titanium dioxide were obtained. The inorganic matrix was modified with K₂Co[Fe(CN)₆] nanoparticles with a size up to 10 nm. The nanoparticles are unaggregated, since they are stabilized by the inorganic matrix. The optimal modifier content, which allows us to obtain large granules of the composite, was found. The modifier nanoparticles loose titanium dioxide increasing its micro- and mesoporosity. Sorption of both cationic and anionic forms of U(VI) under batch conditions was investigated. The modifier improves sorption from one- and multicomponent solutions, especially in weakly acidic and neutral media: the removal degree of U(VI) reaches 80-100 %. When the concentration of U(VI) is 0.02-0.04 mmol dm⁻³, the modifier increases the degree of U(VI) removal from river water by 50 %. Sorption rate is described by the model of pseudo-second order. The modifier slows down sorption of cations, while no effect on the rate of anion sorption has been found. Sorption isotherms are described with Freundlich model. The K₂Co[Fe(CN)₆] nanoparticles decrease energetic heterogeneity of sorption centres.

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Compositions of α -tocopheryl acetate with micellar nanocarriers: preparation, controlled drug release and *in vivo* biological activity

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Micellar drug carriers based on asymmetric diblock copolymers (DBCs) with chemically complementary methoxypolyethylene oxide and polyacrylic acid blocks (MOPEO-b-PAAc) represent in aqueous solutions in the pH range <5 a special micellar structures of the “crew cut” and “hairy” types with a complex “core”. These micelles proved to be very effective, non-toxic, biocompatible and biodegradable nanocarriers for the delivery of a poorly soluble analogue of vitamin E, α -tocopheryl acetate (α -TOCA), in organisms of the sows and piglets. In this work, the mechanisms of formation/release and stability in aqueous and aqueous/salt solutions of *in situ* formed α -TOCA compositions with DBC micelles having different lengths of PAAc “corona” were studied using UV-Vis spectroscopy, static light scattering, dialysis and TEM. The gradual release of a vitamin E analogue from both micellar nanocarriers into an aqueous and aqueous/salt medium under the influence of a concentration gradient of α -TOCA has been proved. The rate and efficiency of α -TOCA release was determined by the structure of DBC micelles.

The possibility of providing of long-term controlled release of α -TOCA in the living organism due to the use of DBC micelles was revealed. Based on *in vivo* tests of the biological action of the composition on pregnant sows, its high bioavailability, rapid absorption, active use in metabolic processes and positive effect on the reproductive qualities of sows compared to pure α -TOCA, were displayed, which improves the safety and productivity of newborn piglets.

Properties of textile materials modified with Ag and Ag/Cu nanoparticles and their virucidal activity in transmission coronavirus model of pigs

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The epidemic situation in the world related to the spread of SARS-CoV-2 virus, and its consequences for human health and economies of countries, encourage the search for ways to reduce the number of viral virions entering the human body and, consequently, reduce viral load on it. One way to achieve this is to find new materials capable of adsorbing and destroying coronaviruses for use in protective clothing and masks. Nanoparticles (NPs) of precious metals and copper, which exhibit high antimicrobial properties, may also have antiviral activity, in particular on the coronavirus strain, as published in the literature.

NPs of silver and bimetallic composite Ag/Cu applied to the cotton surface are extremely effective biocides against a number of bacteria. These materials were used to test virucidal efficacy *in situ*. Samples of the modified fabric were obtained by a simple energy-saving method developed by us: 1) impregnation of a cotton sample in aqueous solutions of silver and / or copper salts; 2) air drying and heat treatment of fabric at 225 °C. After heat treatment, Ag and Ag/Cu NPs with an average size of 60 nm were formed on the cotton surface. Heat treatment can be replaced by irradiating of the impregnated surface with visible light. The obtained materials are characterized by X-ray and optical spectroscopy methods. The presence of the corresponding metal nanoparticles was confirmed by SEM and EDX methods also.

Studies of virucidal activity showed that pure cotton tissue reduces the infectious titer of D52-5 virus by 1.0 lg ID50 by its absorption, the same tissue with applied LF Ag or Ag/Cu composite reduces this titer by 2.0 lg ID50, by destroying the adsorbed viruses. When used in protective clothing and masks, it will significantly reduce the viral load on the human body in contact with coronaviruses, pathogens of dangerous diseases: SARS-CoV, MERS-CoV, COVID-19.

Specific surface, crystallite size of AlB₁₂-nano from products of alumothermy “BN-Al” in vacuum

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The production of metal-ceramic materials for several two decades is associated with the interaction of liquid aluminum and boron nitride [1-3]. The calculation of the heat passing through this reaction shows that it is exothermic. Avoiding oxidation in vacuum, the reaction occurs through the formation of aluminum nitride and aluminum dodeca-boride. In contrast to the liquid state, the process continues until the end, at conditional temperatures of evaporation of aluminum with slight changes in vacuum. The reaction product is a mixture of nanosized AlN/AlB₁₂ powders with a weight ratio of 3/1 ready for baking without grinding [4]. The acid-base properties of the nanosized powder mixture AlN + AlB₁₂, the products of the interaction BN + Al in vacuum, which are used optionally, emit separate phases of aluminum nitride and aluminum dodeca-boride. The yield of AlB₁₂ is ~ 25 %, boron reaches ~ 100 %. The average particle size of the powders according to TEM and (X-ray coherent scattering region) CSR, L (nm) is $L_{\text{TEM}}=110-150\text{nm}$, $L_{\text{CSR}}=51-70\text{nm}$. The average specific surface area of the powder according to BET, TEM and CSR, $S_{\text{BET.m}^2/\text{g}}=21.0-15.0$; $S_{\text{TEM.m}^2/\text{g}}=21.4-15.4$; $S_{\text{OCS.m}^2/\text{g}}=46.1-33.6$; (at 1460 and 1640K, respectively).

Acknowledgements

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Absorption of vitamin B12 on pectin-modified activated carbons

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Carbon adsorbents are widely used as enterosorbents for detoxifying the human body of toxic organic substances. At the same time, this class of adsorbents weakly absorbs ions of heavy metals such as mercury, arsenic and lead. Pectin is an important natural anionic polysaccharide extracted from cell walls of higher plants. This polysaccharide is known as a gelling/thickening agent, emulsifying agent, as well as stabilizer in the food industry. Moreover, pectin can be regarded as an attractive biopolymer material in wastewater treatment that facilitates metal chelation with a backbone of 1,4- α -D-galacturonic acids [1] also pectins have radioprotective effects against radioactive isotopes. Thus, pectin-modified activated carbons (AC) should have an increased adsorption potential against both organic and inorganic toxins.

In order to study the adsorption capacity of adsorbents based on activated carbon and pectins, a series of composites with different ratio AC/apple pectin were prepared and the adsorption of marker substances (vitamin B12, mercury, lead, zinc) was studied. In this paper will be presented the results of the adsorption of vitamin B12 on the obtained composites.

After the modification with pectins, the adsorption parameters of activated carbons decreased significantly from 1800 m²/g to 430-760 m²/g, depending on the AC/pectin ratio. The kinetics of the adsorption process of vitamin B12 ($C_0 = 50$ mg/L) on NM1-NM6 composites was studied at room temperature for 48 h. The data obtained indicate that for samples NM1, NM2, NM3 and NM4 in the first 6 hours about 60-70 % of the adsorbate is immobilized, and 24 hours are sufficient to establish the equilibrium of the adsorption process. For samples NM5 and NM6, the retention kinetics of vitamin B12 is slower, the equilibrium is established after 48 hours of contact and the immobilization rate does not exceed 50 %.

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Elimination of non-biodegradable components from waters using complex drinking procedures

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Provision of safe drinking water is an elementary human necessity and an important human right, especially for maintaining good health. Over 90 % of the aquatic resources of the Republic of Moldova do not meet the requirements for drinking water, containing pollutants of natural or anthropogenic origin. Some of the pollutants can be a health hazard, while others can change the smell, taste and appearance of the water.

The elaboration of water purification technologies represents a complex process that involves the analysis of water quality, the choice of appropriate procedures, the estimation of implementation and maintenance costs. A special class of pollutants are those that in the natural environment are not subject to biological degradation (pesticides, metal ions, polymers, persistent synthetic organic compounds) and that can be removed from water only using complex drinking technologies.

The purpose of the study was to develop a purification scheme of water that does not meet the requirements for drinking water to the following parameters: hardness, content of iron ions, ammonium, nitrates, sodium, sulfates, chlorides and chemical oxygen demand. The study was performed on model water under dynamic conditions, and *o*-nitrophenol and murexide dye were used as synthetic organic pollutants. Both substances are stable in the aquatic environment, and *o*-nitrophenol cannot be removed by the use of oxidants such as sodium hypochlorite or chlorine, which requires the use of additional purification processes such as adsorption on activated carbon. The kinetics and isotherms of adsorption on activated carbon of *o*-nitrophenol and murexide were studied, the results obtained allowed the establishment of optimal conditions for elimination of pollutants under dynamic conditions: the required amount of oxidant, pumping speed, contact time with activated carbon. As a result, a complex water treatment scheme was developed and tested, which includes: oxidation, aeration, ion exchange and adsorption on activated carbon.

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Kinetic and thermodynamic study on adsorption of vitamins B1 and B3 by activated carbons

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This study investigates the vitamins B1 and B3 adsorption performances on commercial (Granucol-FA) and laboratory produced (AC-C) activated carbons (AC). Both activated carbons are predominantly mesoporous (about 70% mesoporous), with a specific surface area of 1360 m²/g (Granucol-FA) and 1385 m²/g (AC-C). The adsorption isotherms were adjusted to Langmuir and Freundlich models, and the adsorption capacity in each system was calculate. The effect of the initial concentration (1-10 mmol/L), contact time (0-1800 min), and temperature (298-318 K) were determined to find the optimal conditions for a maximum adsorption. Equilibrium and kinetic analysis were conducted to determine the factors controlling the adsorption rate, the optimization of various parameters in vitamins adsorption and to find out the possibility of using this activated carbon for food industry. The adsorption mechanism of vitamins onto AC was studied using the first pseudo order and second pseudo order models. The adsorptions kinetic were found to follow a pseudo second order kinetic model. The adsorption isotherms at different temperatures have been used for the determination of thermodynamic parameters such as free energy, enthalpy, entropy, and activation energy of adsorption. The negative free enthalpy (ΔG°) and enthalpy (ΔH°) indicated the spontaneous and exothermic nature of the adsorption process at the examined temperatures range.

Acknowledgements

This research was carried out with the financial support of the institutional project “The reduction of the environmental and health impact of toxic chemicals through use of adsorbents and catalysts obtained from local raw materials” DISTOX, No 20.80009.7007.21.

Hydrogen production by catalytic hydrolysis of sodium borohydride using a platinum catalyst

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Hydrolysis of sodium borohydride is considered as one of the most promising methods for producing hydrogen due to the high yield of hydrogen. Generally, the hydrolysis of sodium borohydride is slow, and a catalyst must be used to reach the sufficient hydrogen evolution rate. In this work, we studied the kinetics of sodium borohydride hydrolysis, catalyzed by nanodispersed platinum, depending on the substrate, to which it was applied.

The kinetic regularities of hydrogen evolution during the catalytic decomposition of a sodium borohydride solution in the flat and cylindrical reactors in a dynamic mode were determined using a volumetric setup.

The catalyst used in the flat reactor consisted of nanodispersed platinum (up to 40 wt.%) deposited on carbon black (XC-72), which, in turn, was immobilized on the surface of the carbon cloth ($1\text{-}2 \text{ mg/cm}^2$). The measured hydrogen evolution rate in such a reactor at 24°C was directly proportional to the rate of the solution circulation through the generator and at the circulation rate of 7.8 ml/min it reached 400 ml/min., what is sufficient for a stable supply of hydrogen to a 30 W hydrogen-oxygen fuel cell. The degree of decomposition of sodium borohydride decreased with an increase of the rate of solution circulation.

For a cylindrical reactor, platinum catalysts were prepared on various substrates. 1). 100 mg of a platinum catalyst (40 %) on XC-72 carbon black was applied to a carbon cloth (50 cm^2), which was then rolled with a 4-mesh polyamide net and loaded into a reactor. 2). 150 mg of platinum was applied to 2 g of activated granular AG-3 carbon by polyol synthesis with reduction by NaBH_4 and placed into the reactor. 3). Platinum was electrochemically deposited on a porous degreased and etched titanium crumb from an electrolyte of 25 g/l K_2PtCl_6 , 100 g/l NaNO_2 , and 20 ml/l ammonia solution (0.915 g/cm^3) at a temperature of 70°C and a cathode current density of 20 mA/cm^2 . Under these conditions, the current platinum yield was about 30 %. The weight of the deposited platinum was monitored gravimetrically. The platinum content on the surface of titanium crumb was $1\text{-}4 \text{ mg/cm}^2$.

It was established that platinized titanium is less active in the sodium borohydride hydrolysis than the catalyst obtained by the polyol method. During the formation of a roll from the carbon cloth with applied platinum catalyst, the latter peeled off. That is why its activity was lower than in the flat reactor.

Biodegradable composite materials based on starch

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Starch is an important ingredient in food and non-food industries (such as paper, plastic, adhesive). Starch is composed of amylose and amylopectin. The widespread occurrence of starch with its biodegradable nature and low cost gave rise to exploitation of starch as a means of improving the biodegradability of inert polymers. Biodegradable composite materials have been produced by mixing polyolefins with biodegradable polymers, obtained from renewable resources by incorporating special additives to the mixture, which accelerate the degradation process.

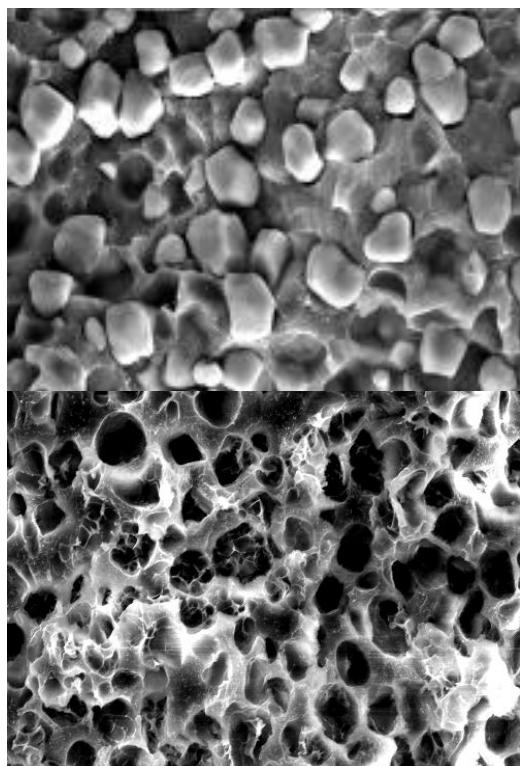


Fig. SEM image of the PP/starch samples before and after composting in natural weathering

In this study, an attempt is made to produce a biodegradable polymer from a polypropylene (PP) and corn starch at different filler content in order to investigate the effect on some properties. The biodegradable composites on base of starch and mixture of polyolefins – polypropylene, polyethylene and ethylene-vinyl acetate are prepared in the form of extrusion bands. It is established that the composite material in the system «starch – polyolefins» contains the particles of filler, disposed in polymer matrix randomly and contains the closed macropores as well. The products after use are exposed by biological decomposition in the conditions of composting in laboratory and nature conditions.

The splitting of electron states in germanium/silicon nanosystem with germanium quantum dots: Theory

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It is shown that electron tunneling through a potential barrier that separates two quantum dots of germanium leads to the splitting of electron states localized over spherical interfaces (a quantum dot – a silicon matrix). The dependence of the splitting values of the electron levels on the parameters of the nanosystem (the radius a quantum dot germanium, as well as the distance D between the surfaces of the quantum dots) is obtained. It is shown that, the splitting of electron levels in the QD chain of germanium causes the appearance of a zone of localized electron states, which is located in the bandgap of silicon matrix. It was found that the motion of a charge-transport exciton along a chain of quantum dots of germanium causes an increase in photoconductivity in the nanosystem [1, 2]. The effect of increasing photoconductivity can make a significant contribution in the process of converting the energy of the optical range in photosynthesizing nanosystems.

It has been established that comparison of the splitting dependence $\Delta E_{ex}(a, D)$ of the exciton level $E_{ex}(a)$ at a certain radius a QD with the experimental value of the width of the zone of localized electron states arising in the QD chain of germanium, allows us to obtain the distances D between the QD surfaces [1, 2].

It has been shown that by changing the parameters of Ge/Si heterostructures with germanium QDs (radii a QD germanium, as well as the distance D between the surfaces of the QDs), it is possible to vary the positions and widths of the zones of localized electronic states. The latter circumstance opens up new possibilities in the use of such nanoheterostructures as new structural materials for the creation of new nano-optoelectronics and nano-photosynthesizing devices of the infrared range [1, 2].

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Sound velocities in graphene-based epoxy nanocomposites

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Recently the introduction of graphene in polymers has made possible the production of a new type of nanocomposite material (NCM) with significantly enhanced mechanical properties [1] manifesting themselves in varying sound velocities (SV). Multilayered graphene platelets (GPLs) are most frequently used in NCM due to the high cost of producing monolayer graphene and its low stability during processing. A further intriguing feature can appear in a periodic arrangement of GPLs that form a repetitive structure composed of two materials with different properties, which is referred to as phononic crystal or metamaterial [2]. The latter research focus on the phononic band edge states with a number of new effects such as guided acoustic wave beam steering [3] and strong SV-dispersion. SV in rod-shaped samples of epoxy-GPL and epoxy-GPL:TiO₂ NCM with varying filler concentrations are measured at frequencies of about 1 MHz utilizing a continuous wave technique and calculated using the effective medium approximation; see Fig. As an overall trend, which is also supported computationally, depositing TiO₂ on GPLs results in decreasing SV, thus making GPL favourable for nano-reinforcement.

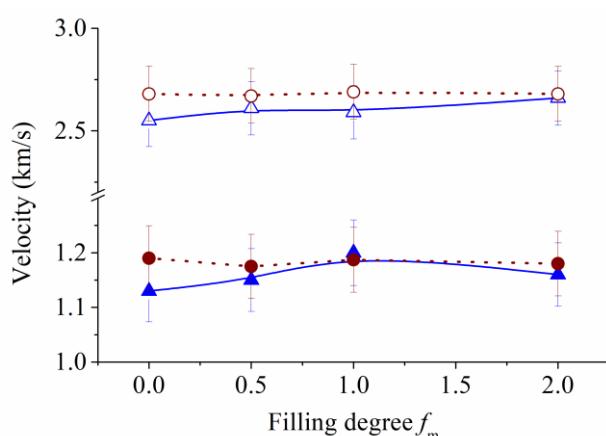


Fig. Phase velocities of longitudinal (open points) and transverse (closed points) ultrasonic waves in epoxy-GPL and epoxy-GPL,TiO₂

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Atomic layer deposition technique (ALD) for obtaining electrode materials for new generation of LIB

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Lithium ion batteries (LIBs) are popular and commonly used for portable electronics and electric vehicles. In the batteries, lithium ions move from the negative electrode through an electrolyte to the positive electrode during discharge, and back during charge. Li-ion batteries use an intercalated lithium compound as the material at the cathode material and typically graphite at the anode.

It is known that the power density of the battery is significantly governed by the diffusion of lithium ions into (and within) the grains of electrode material, and is important for application in electric vehicles. Subdivision leads to great increasing in the area of contact between electrode and electrolyte and decreasing of distances passed by electrons and lithium ions upon diffusion in an electrode material.

One of the most useful ways for improving the electrochemical properties of electrode materials is their surface modification. The atomic layer deposition (ALD) technique is used to coat different metal oxides on the lithium-rich cathode materials. Common coating materials include TiO₂, Al₂O₃, MgO, MnO₂, CeO₂, phosphates FePO₄, CoPO₄ and NiPO₄, fluorides etc.

Using the above approach, the layered lithium-rich Li_{1.2}Ni_{0.16}Mn_{0.56}Co_{0.08}O₂ electrode material modified with Al₂O₃ and vanadium nanoparticles has been synthesized via atomic layer deposition method. The electrochemical performance, surface morphology, and thermal stability of these compositions are investigated to evaluation the effect of the surface modification with different metal oxide nanoparticles on cycling stability and coulombic efficiency. It has been shown that the discharge capacity at 0.1C for the pristine and modified Al₂O₃-NCM samples is 196 and 170 mAh·g⁻¹, respectively, and the capacity retention is 99.4 and 96.8 % for both electrodes. Moreover, the modified by vanadium electrode material demonstrates the high capacity value compared with uncoated material. Thus, Li_{1.2}Ni_{0.16}Mn_{0.55}Co_{0.08}V_{0.01}O₂ return 281 mAh·g⁻¹ at 0.05C while for Li_{1.2}Ni_{0.16}Mn_{0.55}Co_{0.08}O₂ sample the specific discharge capacity at the same current load is only 237 mAh·g⁻¹. Thus, applying the ALD technique leads to obtaining the high electrochemical characteristics of electrode materials.

Impact of the rainwater composition on the wash of soil particles - erosion effect

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Atmospheric pollution and the release of huge amounts of industrial gaseous waste lead to rainwater pollution and its aggression against terrestrial rocks and soils. Specially, due to the trend of aridization in the Republic of Moldova, there is a decrease in the duration of rains and an increase in the flow rate of streams (rain flow per unit of time) of water. In this case, at about the same amount of rainwater the impact investigated is different. The aim of our research was to determine the impact of rainwater chemical composition on the washing of soil particles. A basic criterion for studying the washing of soils by rainwater is to keep the mineral particles in suspended form for a longer time. Soil erosion leads to impoverish the soil as well as to the siltation of lakes and ponds and clogging of other adjacent lands. Following the analysis of the results of a series of rainwater samples collected in different geographical regions of the country, three types of rainwater were modelled: "Moderate" in which the ion HCO_3^- and $\text{CO}_2 \cdot \text{H}_2\text{O}$ predominate, "Acid", in which the anions of strong acids, Cl^- , NO_3^- and SO_4^{2-} predominate, along with HCO_3^- and $\text{CO}_2 \cdot \text{H}_2\text{O}$ and "Ammonia" in which, together with HCO_3^- and $\text{CO}_2 \cdot \text{H}_2\text{O}$, the ammonium ion NH_4^+ predominates. In these models of rainwater, a mixture of CO_2 and air was bubbled. Tests were also made with dilute solutions of these three types of rainwater models. The crushed calcareous rock, the soils of typical chernozem, clay-carbonate and clay-illuvial were researched. The concentration of calcium and magnesium ions, humic substances, chemical oxygen demand were measured. Also, by automatic titration the alkalinity and acidity of the solutions and dispersed systems were determined after 10 and 20 minutes of stirring. The method of gradual crystallization of wet soils was used to investigate the influence of soil stability at sub-zero temperatures. "Acid" type rainwater solubilizes the strongest limestone rock. With the dilution of rainwater, the washing activity of the limestone is best preserved by the ammonia type. In conformity with the resistance to the aggressiveness of the rains, the three types of researched soils are classified in the following series: typical chernozem, clay-carbonate and clay-illuvial. Increasing the pH of rainwater usually decreases the washing of organic matter from the soil. The clay-illuvial type is most affected by rainwater washes containing organic substances. The study of soil changes at low temperatures shows the consolidation of their stability after multiple frosts.

Electrophysical properties of nanocomposites based on carbon nanotubes modified with nickel ferrite

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The design of materials that more efficiently absorb electromagnetic radiation in a wide frequency range is relevant. The combination of magnetic and electrical components enables the possibility of regulating their electromagnetic characteristics, which can be used in the absorption of electromagnetic radiation. Ferromagnetic materials and carbon nanotubes (CNT) can be promising in this direction.

The stoichiometric ratio of iron nitrate $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ and of nickel nitrate $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ solution were prepared and vigorously mixed under magnetic stirring for 2 h at 80°C. The polyvinylpyrrolidone was used as surfactant. Subsequently, the appropriate amount of hydrazine hydrate was added drop by drop into the solution and a black colour NiFe_2O_4 precipitate was formed. Finally, the NiFe_2O_4 nanoparticles were separated by centrifugation and dried in a hot air oven for 4 h at 80 °C. Carbon nanotubes were sonicated for 30 minutes in deionized water. Nanocomposites $\text{NiFe}_2\text{O}_4/\text{CNT}$ were prepared by adding dispersed CNT into salt solution. Further, the synthesis was carried out according to the method described above.

Crystalline structure was determined using the X-ray analysis. The real (ϵ') and imaginary (ϵ'') components of the complex permittivity, the real (μ') and imaginary (μ'') components of the complex permeability of composites at microwave frequencies (9 GHz) were measured using the interferometer and the standing wave meter by an electrodeless method. The immittance meter was used to measure the electrical conductivity (σ) at low frequencies (100 Hz) by two-contact method.

The results of X-ray diffraction study shown that the main reflections synthesized ferrite corresponded to the cubic structure of NiFe_2O_4 (JCPDS № 86-2267). Additional reflections also were observed. These reflections corresponded to the hexagonal structure of Fe_2O_3 (JCPDS 33-664). A halo was observed for composites $\text{NiFe}_2\text{O}_4/\text{CNT}$ in the range of angles $10\text{--}25^\circ 2\theta$, which can be attributed to carbon nanotubes.

For composites with modified CNT, the values of the ϵ' and ϵ'' were 3–4 times higher than for nickel ferrite samples. The values of σ at a frequency of 100 Hz for composites $\text{NiFe}_2\text{O}_4/\text{CNT}$ were 5 orders of magnitude higher than for nickel ferrite samples. For the nanocomposite $\text{NiFe}_2\text{O}_4/\text{CNT}$ (mass concentration of CNT – 2 %), the values were $\mu' = 1.44$ and $\mu'' = 0.15$.

Magnetic layered double hydroxides of Zn and Al, functionalized with complexones, for sorption extraction of ecotoxicants from waters

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Layered double hydroxides (LDHs) functionalized with complexones with magnetic properties are organic-inorganic composite materials that effectively combine the advantages of each component. This makes it possible to obtain unique materials with a high sorption capacity for a wide range of toxic metals-complexing agents, as well as the ability to easily separate dewatered sludge by magnetic separation.

The study of sorption extraction of Cu(II) and Co(II) from aqueous solutions was carried out on samples of nanocomposites based on magnetite and Zn,Al-LDH intercalated with EDTA and citrate ions – Fe₃O₄/Zn,Al-EDTA and Fe₃O₄/Zn,Al-Cit. The synthesis of these sorbents was carried out using ultrasonic treatment of a mixture of functionalized with complexones Zn,Al-LDH and highly dispersed magnetite, which ensured high crystallinity of the materials.

The influence of pH of the model aqueous solution (2.8÷6.0) on the values of sorption of Cu(II) and Co(II) on the studied sorbents was established. At pH of the initial solution (pH₀)≤3.5, both samples are characterized by low sorption capacity. In the range of pH₀≥4.0÷6.0, the maximum sorption of the indicated metal ions from aqueous solutions is observed. In this case, pH of the solution after sorption for Fe₃O₄/Zn,Al-EDTA and Fe₃O₄/Zn,Al-Cit is (6.5-6.7) and (6.8-7.1), respectively. With the extraction of Cu(II), higher distribution coefficients are achieved on both sorbents – 3000 ÷ 5100 cm³/g for Fe₃O₄/Zn,Al-EDTA and 1080 ÷ 1950 cm³/g for Fe₃O₄/Zn,Al-Cit, in contrast to the case of Co(II) – 140 ÷ 180 cm³/g for Fe₃O₄/Zn,Al-EDTA, 280 ÷ 300 cm³/g for Fe₃O₄/Zn,Al-Cit.

The dominant mechanisms for the extraction of Cu(II) and Co(II) are apparently their complexation with EDTA- and Cit-ions of the interlayer space of Zn,Al-LDH, isomorphic substitution of cations in metal-hydroxide layers, and binding with ferrinol (Fe-OH) functional groups of magnetite.

Thus, it has been shown that composites based on LDH and magnetite functionalized with complexones are more promising for the sorption extraction of Cu(II) in comparison with Co(II).

The effect of microwave treatment on the porous structure of zirconium silicate hydrogels

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Zirconium silicates are widely used as high-temperature sorbents and catalyst supports. In order to reducing of energy consumption on development of their porous structure, a comparative study of the effect of hydrothermal (HTT) and microwave treatment on hydrogels of samples was carried out.

Spherical granules of a $\text{ZrO}_2\text{-SiO}_2$ hydrogels, containing ~ 45 % ZrO_2 , were obtained by a continuous sol-gel synthesis from aqueous solutions of ZrOCl_2 , K_2CO_3 and Na_2SiO_3 , at using technology coagulation in a drop. They were washed to remove impurities, converted into the active H-form, dried before measuring the texture parameters, or before that they were subjected to HTT or microwave treatment in an inverter microwave oven at a radiation power of 1000 W. From the shown results on the Figure and in Table, it can be seen that short microwave heating of a pure hydrogel insignificantly changes the structure of the micro-mesoporous sample, but when it is impregnated with NH_4HCO_3 salt, a uniformly mesoporous structure is formed already after 15 min, while at the HTT of pure hydrogel this result achieved in a few hours.

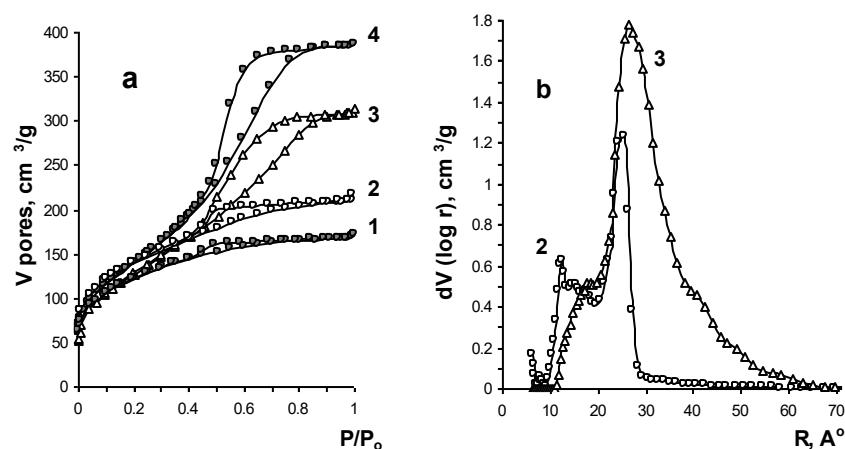


Fig. Isotherms of low-temperature nitrogen adsorption (a) and an example of pore size distribution by radii (b) for samples of Zr-Si hydrogels treated under the conditions given in Table

Table. Texture parameters of Zr-Si hydrogels

Nº	Sample processing	S_{BET} , m ² /g	V_{pores} , cm ³ /g	R_{DFT} pores, Å	R_{Average} , Å
1	Drying at 120 °C	389.3	0.2546	12.37	13.08
2	Microwave 15 min	432.9	0.3386	12.52	13.63
3	NH_4HCO_3 , Microwave 15 min	464.7	0.4874	26.42	20.98
4	15 hours HTT at 270 °C	493.6	0.5976	28.41	24.22

Organosilica materials with improved MCM-41-type structure

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Over the past decades, great efforts have been made in the control of structural characteristics and surface properties of MCM-41-type silica materials to provide their application in catalysis, adsorption, separation, sensing, and biomedicine. In the present work, we studied the ability of amphiphilic organic additives introduced into the templated sol-gel synthesis to affect hexagonal arrangement of one-dimensional mesoporous structure of MCM-41.

Mesoporous silica materials of MCM-41 type with surface silanol, 3-chloropropyl, and 3-aminopropyl groups were synthesized by base-catalyzed sol-gel condensation of structure-forming silanes in the presence of micelles of long-chain quaternary ammonium salts as structure-directing agents and amphiphilic organic compounds as cosurfactants. The effect of amphiphilic organic additives on the formation of mesoporous structure of resulting silicas was estimated by low-temperature nitrogen adsorption-desorption (sorptometer Kelvin-1042) and X-ray diffraction analysis (diffractometer DRON-4-02).

Silicas with 3-chloropropyl and 3-aminopropyl terminated linkers are widely used in design of sophisticated materials. However, analysis of structural parameters proved that involvement of functional silanes in sol-gel synthesis results in decrease of surface area and mesoporous ordering, which is more drastic in the case of (3-aminopropyl)triethoxysilane compared to (3-chloropropyl)triethoxysilane. Introduction of azo dyes, bile acids, and cyclic oligosaccharides in sol-gel synthesis influences mesoporous structure of resulting silicas due to the incorporation inside micelles of long-chain alkyltrimethyl ammonium salts. Solubilization of moderate amounts of amphiphilic organic additives by template micelles driven by electrostatic and hydrophobic interactions has positive impact on formation of open hexagonally ordered mesoporous structure of MCM-41 type.

Regulation of structural parameters of MCM-41-type materials with silanol, 3-chloropropyl, and 3-aminopropyl functionalities, which are widely used in chemical reactions proceeding on silica surface, opens up new opportunities in creation of efficient adsorbents, catalysts, sensors.

C, S-doped TiO₂ nanostructures: synthesis, structure and photocatalytic activity in antibiotics photodegradation processes

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Nowadays, non-metal doped TiO₂ nanostructures are widely investigated as photocatalysts, catalysts, sensors, a wide gap semiconductors in solar cells etc. These materials characterized by specified characteristics (phase composition, electronic structure, morphology, texture), that induce photocatalytic activity elevation. Doped TiO₂ is mainly obtained by sol-gel method, that induce controlling physico-chemical characteristic during synthesis.

The aim of this work was investigation of thiourea/Ti(BuO)₄ ratio in sol-gel system and calcination temperature influence on physico-chemical characteristics of C, S-doped TiO₂ nanostructure and their photocatalytic activity (UV/Vis) |in doxycycline and ceftazidime photodegradation processes.

Doped TiO₂ was obtained by solvothermal sol-gel method with followed calcination. As result, anatase TiO₂ nanoparticle with average crystallite size near 9–11 nm was obtained with thiourea amount increasing. It was found that with an increase in the concentration of thiourea in the reaction mixture, the anatase content decreases together with increase in the particle size, surface area, and carbon and sulfur content. It was shown, that the photocatalytic activity of such materials in doxycycline degradation under UV light irradiation mainly depends on the anatase content and mesopore surface area while under visible light irradiation it also depends on the presence of the interstitial carbonate and sulfate groups. It was found that with increasing calcination temperature, the crystallite size remains in the same range of 9–10 nm, while the morphology of TiO₂ nanoparticles significantly changes, and the anatase content increases from 42 to 95 %. At the same time the nanoparticle size (from 85 to 45 nm), the specific surface area (200–130 m²/g), the mesoporous area (from 170 to 70 m²/g), and the carbon (0.80–0.41 %) and sulfur (1.39–0.89 %) contents decrease. Varying the calcination temperature allows TiO₂ nanostructures to be obtained with a certain balance of these structural-dimensional characteristics that provides high photocatalytic activity in the processes of ceftazidime and doxycycline photodegradation.

As result, C, S-doped TiO₂ anatase nanostructures with average crystallite size in the range 9–10 nm was obtained by solvothermal sol-gel method with followed calcination. It was demonstrated that photocatalytic activity is strongly depends on nanoparticle size, anatase content, surface area, carbon and sulfur content, that controlled by thiourea/Ti(BuO)₄ ratio and calcinating temperature.

Quantum-mechanical study of Cu, Ag and Au slabs

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The unique properties of 2D metal structures are largely determined by the electronic structure. For the targeted synthesis of new nanomaterials with specified characteristics, it is necessary to understand the laws governing the formation of their atomic and electronic structure. However, despite many years of research and an impressive number of works, a theoretical model that would unambiguously describe the features of growth and predict the emerging properties of nanostructures is still far from complete.

Within the framework of the density functional theory in the LAPW + lo approximation (Wien2k package), the tetrahedron method was used to calculate the total and partial densities of electronic states of Cu [111], Ag [111], and Au [111] slabs 1, 2, and 3 atoms thick.

For copper and gold slabs with a thickness of 1 and 2 atoms, there are same general trends in the formation of the DOS curve, and with the transition to thicker samples, the DOS of gold becomes closer to those of silver.

For slabs 3 atoms thick, the shape of the DOS curve is mainly determined by the contributions of the atoms of the outer layers, especially in the long-wavelength part of the spectrum.

It was found that the presence of neighbors determines the shape of the lower part of the valence band of the studied metals.

It is shown that an increase in the number of layers leads to an increase in the intensities of the features in the range of 2-4 eV, which indicates an increase in the population of the valence band in this energy segment.

It was shown that *d*-states make the main contribution to the formation of the DOS curve for all the samples under study. Herewith, with an increase in the number of layers, the DOS curve "stretches", and the greatest response here occurs from the *d*-states associated with the *z* axis.

Features of the formation of a deposit in the arc synthesis of fullerenes

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Because of little attention usually paid to investigation of the deposit in the synthesis of nanostructures, we focused on the study of this product.

As the experiments have shown, in the course of the arc synthesis in addition to the fullerene soot, in which the endofullerenes are formed, a growth, called deposit, as a by-product on the cathode is formed (Fig. 1). It is established, that at evaporation of pure graphite the formed deposit consists of two parts: carbon nano tubes and the graphite mass (Fig. 2). At evaporation of graphite together with any element (in the course of the endo-fullerenes synthesis) the deposit can be formed from two elements and more.

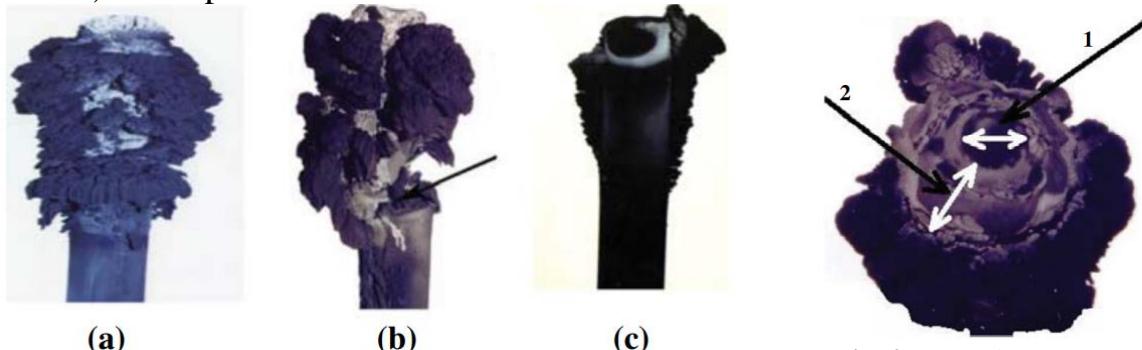


Fig. 1. Cathode (appearance of graphite deposits): (a) deposit, a co-axial cathode, (b) deposit, not a co-axial cathode, (c) anode

Fig. 2. Deposit: 1—Core, 2—shell (deposit bark)

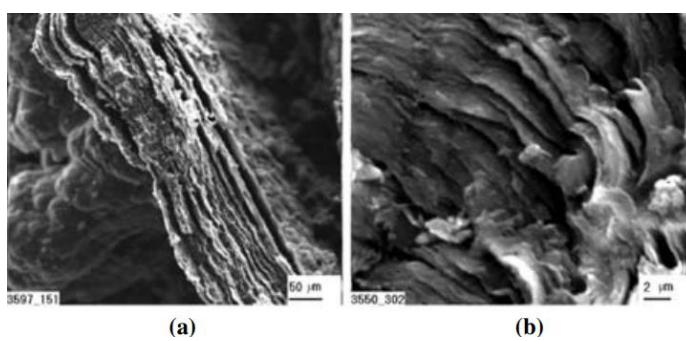


Fig. 3. Deposits envelope

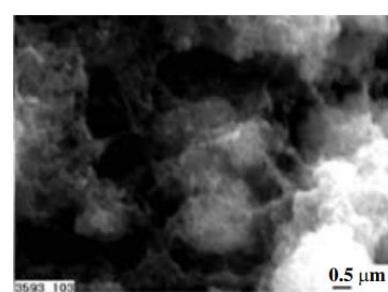


Fig. 4. Deposit core (bundles of nanotubes)

Electron microscopy studies have shown that the deposit shell is formed by layered structures, the planes of which are located perpendicular to the axis of the deposit (Fig. 3 a, b) and densely stacked in a single structure. The core of the deposit is more friable and porous. It consists of conglomerates, oriented along the axis of the deposit, consisting in turn from bundles of carbon nanotubes Fig. 4.

Synthesis of BaO/ZrO₂ nanocomposites by nontraditional methods

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Nanosized composites based on barium and zirconium oxides are newly developed and promising materials which are widely used in various high-tech industries as insulators, capacitors, superconductors. Increased interest in these composites is due to their clear optical and electronic properties. The mechanochemical (MChT for 4 h, air) and ultrasonic (UST for 1 and 2 hours, water medium) treatment were used for synthesis of complex nanodispersed BaO/ZrO₂ compositions with molar ratio of raw oxides 1:1. Obtained results by XRD method show that the isotropic destruction of ZrO₂ without changes in dominant reflex (crystal plane of *m*-ZrO₂ is (110)) and decrease of particle size (Table) is carried out independent of treatment type of BaO/ZrO₂ samples.

Table. Some results of BaO/ZrO₂=1:1 compositions

Parameter	initial	MChT	UST 1 h	UST 2 h
<i>L</i> (m-ZrO ₂ /110), nm	31	16	15	37
<i>S</i> _{BET} , m ² /g	9	12	8	9
<i>V</i> s×10 ⁻² , cm ³ /g	7.71	9.86	11.40	10.24

The DTA/TGA analysis demonstrates three thermal effects. The first an endothermic peak at 80–95 °C is due to evaporation water without weight loss. The second stage of the part removal of the crystal water was observed at 280 °C. The third endothermic effect is between 360 and 560 °C, which is caused by the further removal of the remaining part of the crystal water and the decomposition of BaCO₃. The existence of BaCO₃ was confirmed by FT-IR method also. The structural changes in BaO/ZrO₂ samples were studied by TEM method (Fig.) which also confirms the decrease of particle size.

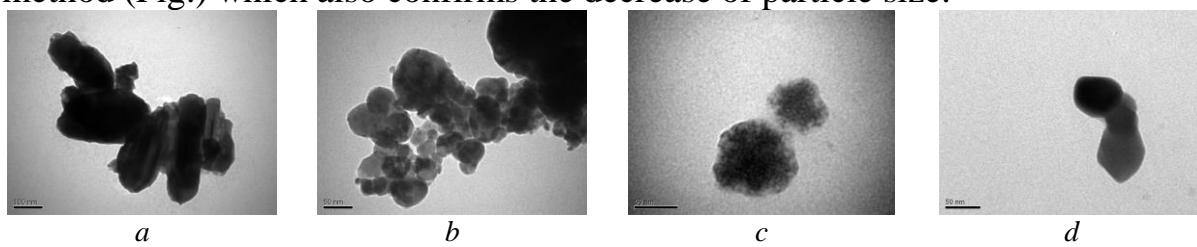


Fig. TEM images of BaO/ZrO₂=1:1 samples: *a* – initial, *b* – after 4 h MChT, *c* – after 1 h UST, *d* – after 2 h UST

Properties of photocured protective coatings on the basis of epoxy-acrylate interpenetrating polymer networks

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Taking into account the depletion of fossil fuels and danger of greenhouse effect, widespread application of environmental-friendly solar energy becomes more and more important. One of the problems concerning solar collectors is the necessity to use heavy and brittle transparent glass coating to protect their surface that not only increases their cost but also – when damaged under weather conditions – requires the exchange of the whole solar element [1]. Photocured materials on the basis of simultaneous epoxy-acrylate interpenetrating polymeric networks (IPNs) with an optical transparency of about 92 % may be proposed both as protective coatings of solar collectors or as sealants for onsite repair of present damaged glass coatings. The sun here can be used as an effective source of UV-radiation for photopolymerization [2].

An aliphatic diepoxide 1-(2',3'-epoxy-propoxymethyl)-1-(2",3"-epoxy-propoxy-methyl)-cyclohex-3-ene (UP-650 D) was used as an epoxy component, difunctional triethyleneglycol dimethacrylate – as an acrylate component, and triphenylsulfonium hexafluorophosphate (50 wt.% solution in propylene carbonate) – as a photoinitiator. Epoxy and acrylate components were mixed in a 100:0, 90:10, 80:20, 70:30 or 60:40 weight ratio, 5.0 wt.% of the initiator solution was added to the mixture. Prevailing content of epoxy component was chosen to create a barrier for oxygen (inhibiting free radical polymerization of acrylate) [3]. Due to this, tack-free coatings were obtained. Aliphatic epoxy component also provides high impact resistance of the coatings, which was measured for steel plates by the Gardner test method (all the coatings withstood the strike of weight falling from a maximum height of the used tester – 50 cm). The acrylate component provides good surface hardness of the coatings and, as we studied before [4], facilitates the epoxide photopolymerization via free-radical-promoted cationic polymerization process [5].

The crosshatch adhesion test has shown that all samples reveal excellent adhesion (100 %) to such substrates as steel, aluminum, glass, and silicone.

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Preparation of meso-macroporous SnO₂ via mechanochemical and microwave treatments and study of its physicochemical, sorption and photocatalytic properties

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The issue of environmental safety determines the search for functional materials, that may be widely used for monitoring and degradation of pollutants. Tin dioxide is one of these perspective materials. The combination of physicochemical parameters of tin dioxide allows to use it as a material for sensors, sorbents and photocatalysts. Therefore, research aimed at regulating and improving the required physicochemical properties using eco-friendly methods is important. The purposes of this work are to study the effect of mechanochemical and microwave treatments of precipitated SnO₂ on its sorption and photocatalytic properties.

Initial SnO₂ has been obtained by heterogeneous precipitation using ammonia. It was subjected to mechanochemical (MChT) and microwave (MWT) treatment under different conditions. Modified samples were tested as materials for sorption of cations under different conditions and photocatalytic degradation of organic pollutants under visible light.

Crystalline structure. All samples correspond to the tetragonal modification of cassiterite (JCPDS (№ 41-1445)). The size of the crystallites (calculated from data of XRD) for samples after MChT and MWT increases, e.g., from 2 to 4 nm for initial and modified samples, respectively.

Porous structure. MChT and MWT of tin dioxide leads to some reduction of specific surface area and increasing the total pore volume, volume of mesopores. The size of mesopores increases from 2.4 to 4.1-4.3 nm. At the same time, peculiarity of milling in water is forming of meso- macroporous structure.

Electronic structure. As a result of MChT and MWT, there is a decrease in the gap E_g (from 4.2 to 3.31 eV for the sample after MChT as a gel), as well as an increase in the absorption of visible light to 18 %.

Sorption studies have shown significant increase the sorption capacity of U(VI), Cs(I) and Sr(II) ions for modified samples to the level of the standard cation-exchange resins and inorganic sorbents. All modified samples exhibit higher *photocatalytic activity* in processes of dyes degradation in aqueous medium under visible irradiation. Rate constants of dye degradation increases 2-3 times. The degree of dyes mineralization is equalled 65-70 %.

Photoluminescence model in macroporous silicon structures with SiO₂ nano-covering and CdS nanoparticles

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Photoluminescence of the oxidized structures of macroporous silicon with CdS-polyethyleneimine nanocoating was determined by the energy distribution of surface states that were dependent on the distance between CdS nanoparticles and their interaction with the polymer environment as well as the CdS-SiO₂/Si boundary. It was found that the maximum photoluminescence intensity was obtained under the following conditions:

1) the maximum electric field strength at the Si-SiO₂ boundary for both previously crude and purified structures of macroporous silicon with CdS nanocoating;

2) increasing the flow of electrons from the silicon matrix towards the CdS nanocrystals;

3) an increase in the residence time of electrons at the Si-SiO₂ interface, which significantly reduces the rate of non-radiative recombination at the CdS-SiO₂ interface.

The efficient light-emitting structures were fabricated on the basis of oxidized macroporous silicon structures with CdS nanocrystals. It was established that the maximum electric field strength at the silicon - nanocoating interface corresponded to the maximum photoluminescence intensity. The quantum yield of photoluminescence of CdS nanoparticles on the surface of oxidized macroporous silicon with the optimal thickness of the SiO₂ layer was increased in 3-4 times reaching 28 % during the first 2 weeks due to the evaporation of water molecules from the nanoparticle layer in the polymer (Fig.). During further storage of the samples, the spectrum and quantum yield of photoluminescence were almost unchanged.

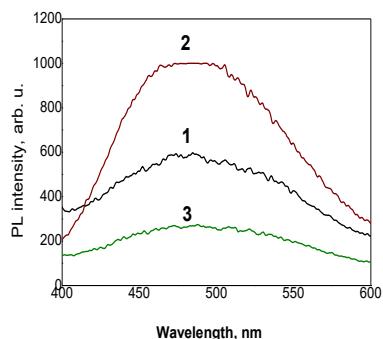


Fig. Spectral dependences of photoluminescence intensity of macroporous silicon structures with CdS nanocoating 1 week after its application and oxide thickness of 20 nm at macropores depth: 1 - 37 μ m, 2 - 75 μ m, 3 - 120 μ m

Synthesis of ZnO nanorods for electronics and solar cells applications

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Currently, a large number of semiconductor devices with use of nanostructures of zinc oxide of in the form of nanowires, nanocores, nanotapes, etc. are actively developing [1]. In this work, according to the proposed procedure, the growth of zinc oxide nanostructures took place in two stages. The seed layer was applied to the substrates by sol-gel method. The hydrothermal method, which has been used to form one-dimensional nanocrystals ZnO on the seed layer, is carried out at low temperatures, does not require expensive equipment and is easily scaled for mass production. The conductivity of the nanostructures is ZnO increased by alloying, and the oxidation resistance of Ga and the proximity of the ion radius to the radius of Zn is decisive for the use of Ga as an alloying element. Images (Fig.) obtained using a scanning electron microscope showed that the morphology of the synthesized nanostructures depends on the concentration of precursors, the time and temperature of growth, the pH of the solution and doping. ZnO nanorods located at an indirect angle to the surface of the substrate can be used as nanodiodes and in solar cells.

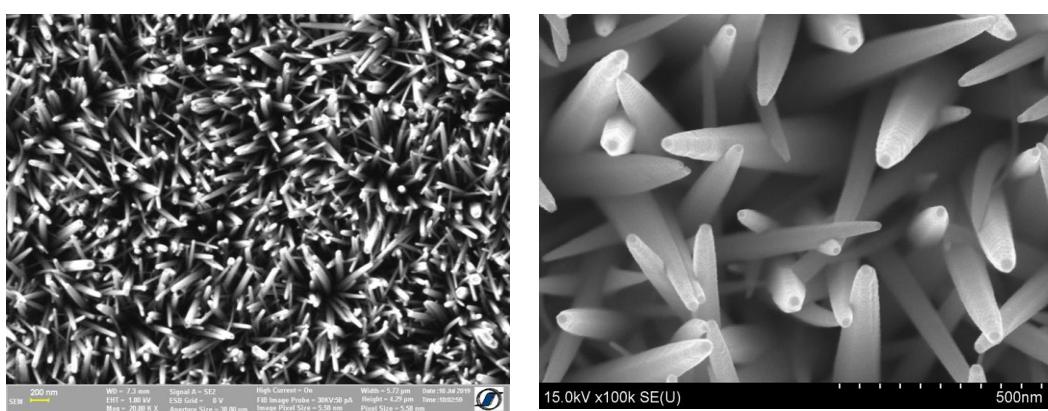


Fig. SEM image of ZnO structures on glass substrates

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Biocoal from walnut shell and usage in naproxen removal

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Naproxen is one of the most widely used non-steroidal anti-inflammatory drugs group in the world [1]. Nowadays, the frequency of this and similar uncontrolled use, drug residue in waste water has increased. Low values of drug residues in wastewater are an important problem for humans and the environment. These drug residues in the waters adversely affect aquatic organisms and may prevent the development of fish. In addition, it harms the skin of aquatic creatures and affects their food and drinking water [2]. For these reasons, it is an important issue to remove drug residues from water.

In this study, the shells of walnut fruits of the type Çetnir (*Junglans hindsii*), which are agricultural waste, were used. Biochar was obtained by burning walnut shells at $700 + 700$ °C pyrolysis temperature for 4 h + 4 h. Later, the obtained biochar was used as an adsorbent in the removal of naproxen, which is classified as a contaminant in water. Characterization of crude biomass and biochar obtained by pyrolysis method was performed using FTIR, TGA-DTA, SEM, EA, BET and XRD techniques. In order to determine the conditions in which the adsorption capacity is maximum in batch adsorption experiments; adsorbent amount, analyte concentration, pH, time and temperature parameters were examined. The appropriateness of the equilibrium data to the Langmuir and Freundlich isotherm models was investigated. In addition, the kinetic model of the adsorption process was determined and the model constants and correlation coefficients were calculated.

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Synthesis and structure of nanosized rutile titanium dioxide

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The use of nanostructured forms of titanium dioxide TiO_2 in modern technology requires further improving the methods of their synthesis. To obtain the rutile form of TiO_2 , we used a “soft chemistry” approach, which allows us to reduce time and energy costs. This method is based on the slow hydrolysis of dilute TiCl_4 solutions, in which the formation of rutile TiO_2 occurs at the moment of precipitation.

The purpose of this work was to identify the correlation between synthesis parameters and physico-chemical properties of TiO_2 .

The physico-chemical properties of the materials obtained were characterized using X-ray diffraction (XRD), porosimetry, and scanning electron microscopy (SEM) methods. After heat treatment, the XRD patterns of the samples obtained correspond to TiO_2 with the rutile structure and crystallite sizes of 6-10 nm. The specific surface area ($S_{\text{sp.}}$) of the starting TiO_2 is $203 \text{ m}^2/\text{g}$. Prolonged heat treatment at the temperatures of 350 and 470°C leads to a drop of $S_{\text{sp.}}$ to $30\text{-}60 \text{ m}^2/\text{g}$. According to the porosimetry data, the synthesized TiO_2 samples have mesoporous structure with dominant pore size of 2-5 nm. Using SEM (Fig.), it was found that the particles of the obtained materials have a spherical shape and are nanosized.

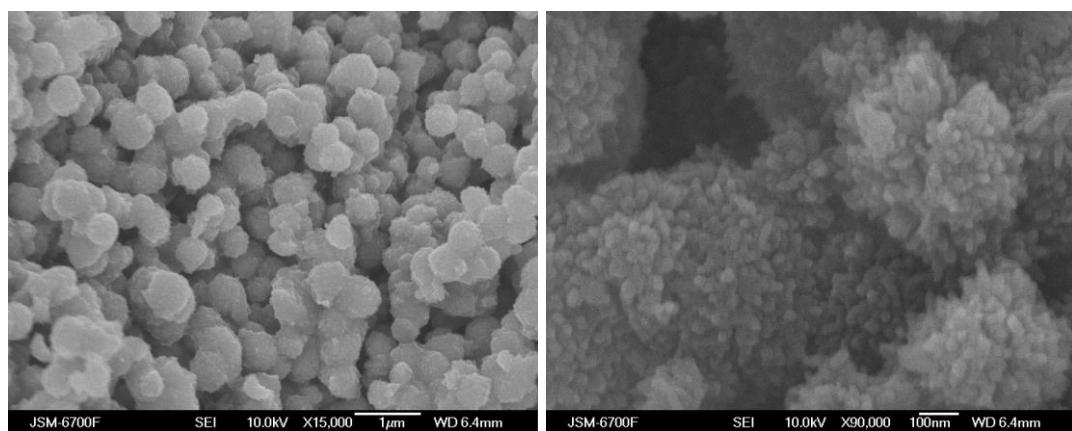


Fig. SEM micrographs of rutile TiO_2 at different magnification

The results obtained in this work can be used in the development of new catalysts or electrode materials for chemical current sources and in other applications.

Simultaneous photocatalytic oxidation of substituted benzyl alcohols and H₂ evolution over crystalline graphitic carbon nitride under visible light

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Crystalline graphitic carbon nitride (CGCN) was synthesized by aerobic thermal treatment of the pristine g-C₃N₄ in a melt of lithium and potassium salts [1]. The photocatalytic properties of the samples have been studied in the processes of molecular hydrogen evolution from aqueous solutions of different benzyl alcohols (BA) under visible light, which allows to obtain hydrogen and valuable products of organic substrates photoconversion. It was established that the efficiency of processes significantly depends on the nature of substituents in the molecule of benzyl alcohol. Thus, in the presence of 4-nitrobenzyl alcohol, hydrogen was not formed at all. For other alcohols, the hydrogen evolution rate increases along the following order: Cl- < H- (unsubstituted BA) < methyl- < methoxy- (Fig., a). The highest rate of hydrogen evolution was achieved in aqueous-acetonitrile solutions acidified with 0.1 HCl, at 40 °C at an optimal content of 4-methoxybenzyl alcohol, which is 720 μmol h⁻¹ g⁻¹ (quantum yield $\gamma = 22\%$ at 405 nm) (Fig., b).

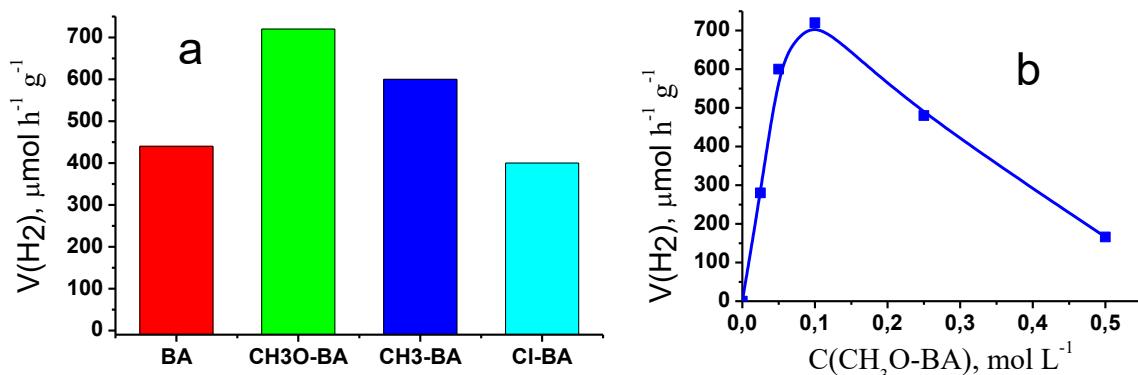


Fig. 1. The dependence of the activity CGCN in photocatalytic hydrogen production under visible light on the nature of organic substrate (a) and the 4-methoxybenzyl alcohol content (b)

The obtained photocatalysts are active under visible light, stable, do not contain toxic and high-value metals and can be used for the development of practically important systems for the simultaneous production of hydrogen and value-added organic products.

1. V.V. Shvalagin, G.V. Korzhak, S.Ya. Kuchmiy, M.A. Skoryk, O.V. Selyshchev, D.R.T. Zahn, J Photochem. Photobiol. A: Chem. **390** (2020) 112295.

Influence of the rare-earth nitrate solutions concentration on the structure formation of perovskite-type oxide phases

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One of the promising areas of modern materials science is the development of technologies for production of transparent functional ceramics from poorly investigated nanopowders of complex oxide phases with perovskite-type structure.

Adsorption-structural studies of precursors synthesized by heterogeneous precipitation from nitrate solutions of REE Ln^{3+} (La^{3+} , Lu^{3+} , Yb^{3+}) showed that at nitrate concentration of 0.1 mol/l and equal other conditions, nanodisperse, mesoporous powders with high specific surface S_{BET} ($152.2 \text{ m}^2/\text{g}$) and large volume of mesopores ($0.26 \text{ cm}^3/\text{g}$) of fine size 4.8 nm, were formed. Increasing the concentration of Ln^{3+} nitrates to 0.25 mol/l promotes the formation of almost non-porous precursors with a defective surface and S_{BET} $4.2 \text{ m}^2/\text{g}$. According to XRD, the precursors have a predominantly amorphous structure. After thermal decomposition of the precursors nanodisperse, mesoporous powders with S_{BET} of 20 and $13 \text{ m}^2/\text{g}$ and particle sizes of 37 and 55 nm, respectively, are formed. XRD shows the content of additional phases, the number of which increases with increasing concentration of nitrate solutions. Thus, the concentration of nitrate solutions is one of the influencing factors in obtaining LaLuO_3 nanopowders with a perovskite-type structure.

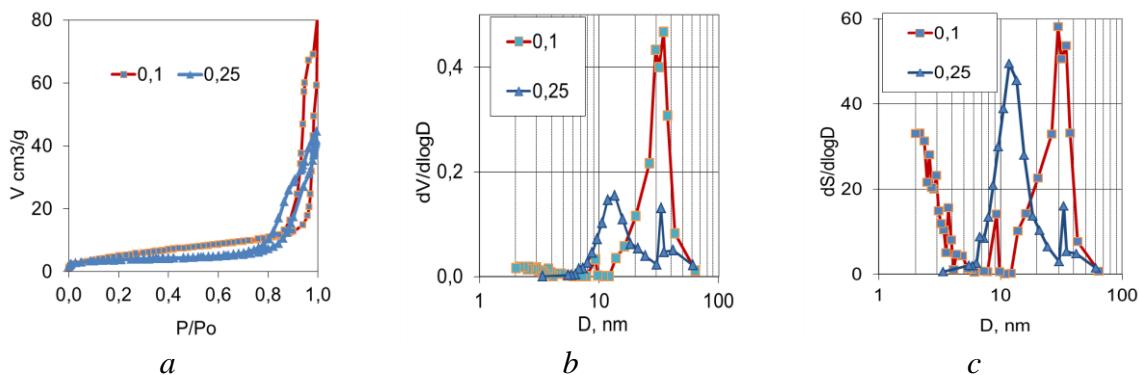


Fig. Nitrogen sorption isotherms (a) and differential size distributions of mesopores volumes (b) and surfaces (c) on the final products of thermally decomposed precursors

Effect of graphene filler oxidation on the thermal destruction of epoxy-graphene composites

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Comparative analysis of the thermal destruction of epoxy resin composites with multilayer unoxidized and oxidized graphene nanoparticles is carried out. Size of the basal surface of particles was about 5 μm , the thickness of the lateral surface was about 50 nm and the number of graphene layers was about 100. The filling of the polymer matrix did not exceed 5 wt.% and excluded the formation of graphene agglomerates. The matrix thermal destruction was investigated using method of thermoproduced desorption mass spectrometry. Thermal desorption of polymer structure atomic fragments was recorded in the range m/z of 15 – 124 and the temperature range up to 800 °C.

The aim of this work was to determine the effect of graphene electronic subsystem on the polymer matrix thermal destruction by varying the surface electronic state of unoxidized particles using oxidation and the formation of surface atomic dielectric layer consisting of oxygen. In the epoxy composites with unoxidized graphene thermal transport to the surface of filler particles is carried out by a phonon flux along polymer chains. At interface the thermal transport is divided into electron and phonon heat fluxes that transfer heat to the bulk of particles. When heat is removed by the electronic subsystem, the temperature of polymer structure fragments fastened on the surface centers decreases and latter leads to an increase in the thermal stability of epoxy composites. With a formed oxide layer on the surface of particles, the electronic subsystem of graphene does not participate in thermal transport, and the phonon heat flux from the polymer through the oxide layer enters to the volume of graphene particles. In this case, the temperature on the oxide layer surface does not experience an abrupt decrease that leads to an increase in the composite thermal decomposition.

It has been established that exhibition of dielectrical atomic layer on the surface of graphene particles leads to an increase in the thermal destruction of composites. The effect of electronic subsystem is distinctly revealed in a growth of the thermal stability of light atomic fragments with $m/z < 55$ and a content of non-oxidized filler $C_n \leq 1$ wt.%. With an increase in the graphene content, the influence of the electronic subsystem on the thermal stability of composites weakens.

Methyl silica/gelatin composite system and its sorption properties

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Silica adsorbents are widely used in medicine and pharmacology due not only to their developed specific surface area, but also the presence of hydroxyl groups, which are the adsorption centers of water and other substances. When the silica surface interacts with the aqueous medium, a film of strongly bound water is formed, preventing the adsorption of average molecular weight. This can be avoided by partial or complete hydrophobization of the surface. However, in this case there is a problem of transferring hydrophobic substances into the aqueous medium. To eliminate this, gelatin as co-adsorbate was used, that adsorbs on the hydrophobic surface, facilitates the water wetting process. Getting into the gastrointestinal tract, gelatin is easily broken down by organism enzymes, releasing the sorbent surface for sorption of toxic substances.

Therefore, the aim of this study was to study the sorption of the anionic dye Congo red by the composite system based on methyl silica and pharmaceutical gelatin.

Methyl silica (AM-1-300, Kalush, Ukraine) and pharmaceutical gelatin (Belgium) were used in the work. Adsorption of Congo red dye (CR) ($M = 697 \text{ g/mol}$) (Reapharm) on the surface of the composite system was performed under static conditions. Composites were prepared in two ways: 1) grinding dry mixtures of AM-1 and gelatin in a ratio of 1:1 with the water addition of 30 wt.%; 2) preparation of 2 % gelatin gel, which after gelling was ground with methyl silica, resulting in the formation of a homogeneous suspension. Both samples were dried at room temperature for 48 hours. To portions of the composites (50 mg) was added 5 ml of CR at a concentration of 0.03 mg/ml and kept for 2 hours. It was found that for composites 1 and 2 the adsorption amount of CR was 2.81 and 0.24 mg/g, respectively, and the degree of dye extraction from the solution was 94 and 80 %.

Thus, composites based on methyl silica and gelatin show significant adsorption activity against Congo red dye from aqueous solution. The investigation of the gelatin interaction with Congo red confirms the effectiveness of this process. Hence, on the basis of hydrophobic silica modified with gelatin, multi-purpose adsorbents can be created to remove hydrophobic and hydrophilic toxins and molecules of average molecular weight.

Changing the profile of phenolcarboxylic acids in barley plants at seed treatment with a nanocomposite complex bacterial preparation Azogram

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Barley (*Hordeum vulgare*) is a valuable cereal crop, its cultivation is severely limited by various abiotic and biotic stress factors. Their increasing action initiates an increase in plant cells of the level of reactive oxygen species (ROS), which by damaging a number of biologically active molecules, cause a violation of ontogenesis in general. One of the promising areas for increasing the stress resistance of barley plants is the use of highly effective microbial preparations. The mechanism of the stress tolerance formation of plants by means of biological preparations is closely connected with metabolites of bacteria. Some of them are triggers, which activate a cascade of biosynthetic processes in a plant organism, that increase resistance to the harmful effects of ROS. One of such processes may be the activation of the synthesis of phenolic compounds in the phytoorganism.

It was found that the treatment of barley seeds varieties Virazh (Ukraine), Burhant (Mongolia), Copeland (Canada) by the stress agent (H_2O_2) and post-treatment by the nanocomposite complex bacterial preparation Azogram significantly affected the profile of phenolcarboxylic acids of plants.

The hydrogen peroxide treatment of the barley seeds inhibited the synthesis of phenolic acids in plants of Burhant variety by 268.831 $\mu\text{g}/\text{mL}$ and Copeland variety by 86.487 $\mu\text{g}/\text{mL}$, according to the control. Syringic acid in methanolic extracts of barley plants of the Burhant and Virazh varieties was not identified.

The concentration of phenolic acids increased by 13.632 $\mu\text{g}/\text{mL}$ only in plants Burchant variety, compared with the content of these compounds in stressed plants of the same variety at post-treatment of barley seeds with by Azogram. However, the stimulating effect of the biological preparation on the content of phenolic acids in plants of the two other varieties of barley was not detected. With all identified phenolcarboxylic acids were present in the qualitative composition. Among them 4-hydroxyphenylacetic, chlorogenic, caffeic, benzoic, p-coumaric, trans-ferulic, sinapic, trans-cinnamic acids, as well as syringic acid, the concentration of which was increased.

Doxorubicin release from the surface of iron oxide nanoparticles in the presence of DNA

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Using nanoparticles as carriers of drugs is a developing trend in pharmaceutical therapy [1]. An essential stage in the nanocarriers design is the study of the nanoparticle effect on the drug interaction with the target molecule. In this work, we investigated the effect of the superparamagnetic iron oxide nanoparticles (SPION) on the anticancer drug doxorubicin (DOX) interaction with the calf thymus DNA. The SPION surface was functionalized previously with the sodium citrate to increase the nanoparticle loading with the drug [2].

Spectrophotometric titrations were performed in binary (SPION-DOX, SPION-DNA, DOX-DNA) and ternary (SPION-DOX-DNA) systems. The experimental data sets were analyzed by the MCR-ALS algorithm (multivariate curve resolution). It allows one to obtain the pure spectra of all absorbing particles in the system and determine their relative contributions to the measured spectra. The calculated data were used to plot the experimental binding isotherms. These dependencies were fitted by Langmuir and McGee equations to determine the equilibrium parameters of DOX binding to SPION and DNA.

It is found that negatively charged SPIONs almost do not interact with DNA. The calculated binding constants of DOX with SPION and DNA are $1.5 \cdot 10^4 \text{ M}^{-1}$ and $4 \cdot 10^4 \text{ M}^{-1}$, respectively. Also, for the SPION-DOX-DNA ternary system, the dependences of the concentration of DNA-bound doxorubicin on the total DNA concentration are obtained. With increasing DNA concentration, a gradual release of DOX molecules from DOX-SPION complexes with further binding to DNA is observed. At high DNA concentrations, almost all DOX molecules are bound to DNA. Thus, SPIONs are promising carriers of DOX. They do not interact with DNA, and their use does not require increasing the drug dose to achieve a therapeutic effect.

The authors are grateful to Prof. A. G. Belous for providing the iron oxide nanoparticles samples.

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2. E.G. Bereznyak, E.V. Dukhopelnykov, D.A. Pesina, *et al.*, *BioNanoSci*. **9** (2019) 406.

Mesoporous silica- and titania-based films as substrates for LDI-MS spectrometry

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The search for new nanostructured materials promising as substrates for SALDI is an important area of research in mass spectrometry. Nowadays matrixless methods of desorption-ionization from the surface of porous silicon, silicon nanorods, hybrids films made of nanoparticles on the silicon surface are introduced. In this work transparent mesoporous TiO_2 , $\text{TiO}_2/\text{SiO}_2$, SiO_2 films, and films doped with Ag nanoparticles, on the glass plates were synthesized via template sol-gel method. Prepared substrates were used for parallel studies of low-mass organic substances by electron spectroscopy and laser desorption/ionization methods. Thermal and mechanical stability, chemical purity of annealed sol-gel films ensure the absence of background lines in the mass spectra, even at the maximum laser power for the device used. Combination of inert film coating and metal component has the significant advantages over other matrix free approaches as it provides the inclusion size checking capability and allows of reducing aggregation problem. The active components of the film that affects ionization are silver nanoparticles with a size of 5-12 nm, characterized by the presence of localized plasmon resonance. Using such materials, the test compounds can be introduced into a mass spectrometric experiment in a crystalline, condensed-on-substrate state, adsorbed, or chemically bound to the surface groups of the substrate. The presence of pores in the substrate material increases the capacity of the substrate on the sample, provides a uniform distribution of the compound in the plane of the irradiated spot during sample preparation. The active components of the TiO_2 films with photoinduced superhydrophylicity that affects the ionization of the test substance are nanosized anatase particles that absorb light in the UV range. So TiO_2 substrates make it possible to simulate both reductive and oxidative reactions directly in a mass spectrometric experiment. Addition of Ag nanoparticles into mesoporous SiO_2 , $\text{SiO}_2/\text{TiO}_2$ and TiO_2 films lead to increase the peak intensity in LDI spectra of adsorbed molecules. Ag peaks (m/z 107, 216 and 323) do not interfere with analyte peaks. SiO_2 films as a matrix are preferred as a sufficiently inert material that prevents active oxidation of Ag. The efficiency of the ionic yield of the analyte depends on a number of physical characteristics of nanoparticles, the ratio of the number of NP to the number of analyte molecules, the characteristics of adsorption bonds.

Spatial structure and IR spectral manifestation of tin impurity sites in titanium dioxide

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A promising material that has a high transmission in the visible range and electrical conductivity can be developed on the basis of titanium dioxide modified with tin dioxide impurities. The work is devoted to measuring and calculation of vibrational spectra of pure and tin-containing titanium dioxide. Clusters $Ti_{14}H_{22}O_{39}$ containing 1, 2, or 3 impurity tin atoms were considered (Fig. 1). The IR spectra were recorded on a single-beam IR Fourier spectrometer Thermo Nicolet Nexus FT-IR (Germany). The prepared samples were mixed with freshly calcined KBr at a ratio of 1: 4.

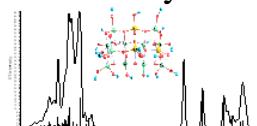


Fig. 1.°Partial geometry and IR-spectrum of the anatase model with three Sn atoms

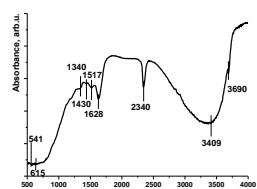


Fig. 2.°Experimental spectrum of Sn/TiO₂ sample

The calculations were carried out within harmonical approximation in the framework of the cluster approximation using the density functional theory B3LYP method and the basis set 6-31G (d,p), using the PC GAMESS software package (FireFly version 8.2.0 by A. Granovsky). From a comparison of the experimental spectra with the results of calculations, it follows that impurity tin atoms appear in the range of bending vibrations of Sn-O-Sn about 615 cm^{-1} , in contrast to vibrations of Ti-O-Ti about 500 cm^{-1} . In the range of stretching vibrations of OH-groups $3500\text{-}3700\text{ cm}^{-1}$, Ti-OH and Sn-OH groups are practically indistinguishable.

In the spectra of samples (Fig. 2) in the region of absorption of $\nu(OH)$ vibrations of 3300 cm^{-1} , a wide intense band is observed, which is attributed to the stretching vibrations of bonds in crystallization water and absorption at 1628 cm^{-1} , which refers to bending vibrations in sorbed water. Absorption bands of free OH groups at 3690 cm^{-1} and of bound OH groups at 3409 cm^{-1} are also observed. A peak at 615 cm^{-1} corresponds to Sn-O-Sn vibrations, and at 541 cm^{-1} to Ti-O-Ti ones. The spectrum also shows an absorption band with a maximum of 2340 cm^{-1} , which corresponds to carbon dioxide physically sorbed on the surface of the composite.

Effect of heat treatment on the properties and form factor of ZTA powder produced by hydrothermal synthesis in alkaline medium

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In recent years among the materials for various purposes (instrumental, structural, functional), considerable attention is paid to ZTA-composites, in which the α -Al₂O₃ matrix is reinforced by particles of tetragonal ZrO₂-based solid solution (T-ZrO₂).

The initial powder composition (wt.%): 90 Al₂O₃ – 10 ZrO₂(Y₂O₃, CeO₂), was produced by hydrothermal synthesis in an alkaline medium. The composition of the solid solution based on ZrO₂ is (mol.%) 90ZrO₂ - 8CeO₂ - 2Y₂O₃. To investigate the physico-chemical properties evolution of the nanocrystalline powder, its thermal treatment in the temperature range of 400 – 1450 °C was performed. The properties of synthesized powders were characterized by scanning electron microscopy (SEM) and X-ray diffraction (XRD). The AMIC program ("Automatic Microstructure Analyzer") was used for the data processing of the powders morphology.

According to XRD, boehmite γ -AlO(OH) and metastable cubic ZrO₂-based solid solution (F-ZrO₂) were formed in 90AZG after hydrothermal synthesis. The heat treatment of 90AZG powder was accompanied by decomposition of γ -AlO(OH) and phase transformations both Al₂O₃ and ZrO₂.

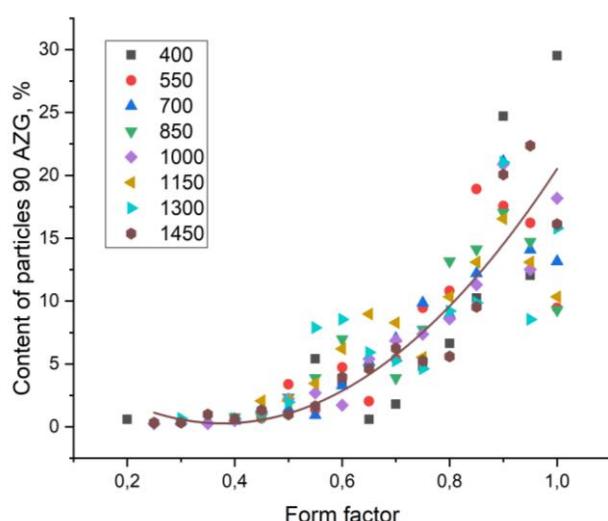


Fig. Form factor of 90AZG powder in the process of heat treatment

The morphology of soft agglomerated powders varies topologically uninterruptedly. Changes in the form factor of nanocrystalline 90AZG powder during thermal treatment are shown in Fig. The similarity of the change in the form factor indicates that the effect of "topochemical memory" of ceramics is already manifested in the thermal treatment of 90AZG powder.

About mistakes in calculation of thermodynamic parameters of adsorption

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Nowadays adsorption method for wastewater treatment has attracted substantial attention from the scientific community. The number of scientific publications in the field of adsorption studies is increased. There are great amount of articles containing thermodynamic calculations of adsorption because thermodynamic parameters are an indispensable component of predicting adsorption mechanisms. However, there are articles containing mistakes related to the study of adsorption thermodynamics.

The purpose of this paper is to identify and analyse mistakes in current scientific publications and prevent of such mistakes in studying of adsorption thermodynamics.

The Gibbs energy change (ΔG°) can be computed using the following equation:

$$\Delta G^\circ = -RT \ln K^\circ \quad (1)$$

The enthalpy change (ΔH°) and entropy change (ΔS°) are determined from the slope and intercept, respectively, of a plot of $\ln K$ versus $1/T$.

The units of ΔG° are J/mol in the International System of Units, and the equilibrium constant K° in Eq. (1) must be dimensionless. This is in accordance with the recommendation of the IUPAC. Values of the thermodynamic parameters is directly dependent on accurate determination of the equilibrium constant K° . In the literature, the thermodynamic parameters calculate using values of equilibrium constant as constant derived from adsorption isotherms of Langmuir, Freundlich and Henry or as the partition coefficient. However, the equilibrium constant K° must be dimensionless. The partition coefficient is dimensionless, but according to the USEPA, the partition coefficient is only appropriate for calculating the thermodynamic parameters if the initial used adsorbate concentration is low. It should also consider that the linear regression coefficient R^2 for a plot of $\ln K$ versus $1/T$ must be high.

Thus, it was calculated the equilibrium constants using numeric examples and shown the flaws of the thermodynamics calculations when the value of K° is wrongly calculated. In a number of articles the incorrect calculations of the equilibrium constant led to an incorrect interpretation of the obtained adsorption results.

Physicochemical properties of the “water - underwater sediment” system of a lake in the process of eutrophication

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The purpose of the study was to reveal the state of the dispersed aquatic systems with different fractions of underwater sediment from the southwest shore with reeds of the Ghidighici Lake, located not far from Chisinau. The role of the processes leading to the eutrophication of a lake in the geographical-climatic conditions specific to the Republic of Moldova was elucidated. In this research 7 fractions were obtained. A number of physicochemical methods have been used, including infrared spectroscopy, thermal analysis, X-ray diffraction (phase X-ray analysis) and automatic acid-base titration. The separation of each fraction was achieved following the sedimentation time, based on the principle of the difference in density of particles of diverse mineralogical nature. Taking into account their chemical composition and specific properties, the fractions were prepared, conventionally named as: 1) coarse sandy, 2) semi-heavy sandy, 3) clay-sandy, 4) average clayey, 5) coarse organic, 6) average organic, 7) fine clay (slightly peptizing). Two organic fractions made up of plant remains, which developed in the Ghidighici Lake due to the process of eutrophication. The organic fractions from the underwater sediment in the lake were separated from the mineral part. The existence in the underwater sediment samples of different minerals, characteristic of the respective geographical areas: quartz, montmorillonite, ilite, carbonates and others was found. Suspended particles have been shown to have a much higher ion exchange activity than soil particles. As a result of the washing process, a selection of minerals takes place with a higher ion exchange capacity and a higher degree of dispersion/wetting, as in the case of montmorillonite. The highest buffering capacity shows fraction 4 (medium clayey). This fraction, according to the thermogravimetric assessment, contains a considerable amount of organic substances, mainly humic, forming an organo-mineral complex. The average organic fraction 6, humidified, also has a significant buffering capacity. A special case is represented by the peptized fraction 7, in which well-loosened minerals predominate, slightly hydrated from the group of clays, such as expandable aluminosilicates, in which the processes of exchange, combination and complexation of ions proceed easily. The structures of this dispersed system, charged with negative electrical charges (anionic particles) form a stable complex with N-cetylpyridine, with dimensions of flocs of the same order.

Synthesis of g-C₃N₄ supported ultrasmall silver nanoparticles for the application in photocatalysis

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Graphitic carbon nitride (g-C₃N₄) is a 2D metal-free polymeric material based on carbon, nitrogen and residual hydrogen atoms, with remarkable chemical and electronic properties. Such important properties, as high thermal, physical, chemical and photochemical stability, allow to apply this metal-free semiconductor for solar cell productions, imaging, sensing of some compounds. This highly ordered g-C₃N₄ is suitable support for the synthesis of metal single atoms and ultra-small particles. Silver nanoparticles (NPs) are active and tend to coalesce during preparation and catalytic process. Therefore, the using of host inert matrix promotes the high dispersion of metal NPs, prevents the aggregation and stabilizes them. In our work we report the obtaining ultra-small Ag NPs by chemical reduction of Ag⁺-doped g-C₃N₄. The advantages of chemical reduction method of Ag NPs supported g-C₃N₄ are simplicity, cleanness, convenience, controllability in situ reduction. As shown on HRTEM image of Ag NPs-doped g-C₃N₄ (Fig.), Ag NPs with size about 1 nm are widely and uniformly distributed on the surface of g-C₃N₄ nanosheets. Ag NPs decorated g-C₃N₄ exhibited improved photocatalytic activity for organic dye and antibiotics degradation under visible light irradiation.



Fig. HAADF-TEM image of Ag NPs-doped g-C₃N₄

Modification of implant surfaces with tricalcium phosphate and noble metal nanoparticles by EBPVD

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The emphasis in the modern regenerative approach to bone treatment and replacement is placed on replacing biomaterial with growing bone tissue. In this case the biomaterial acts as an active source of elements for bone tissue building. Furthermore, effective osteostimulating action, acceleration of the processes of accretion and growth of new bone tissue into the implant requires the porosity of biomaterial.

The objects of this study are widely used biocompatible materials - Ti, and a bone tissue analogue - $\text{Ca}_3(\text{PO}_4)_2$. Technologically the porosity was formed by the growth of titanium in the vapor of the NaCl additive.

Thick - 20...150 μm Ti films containing 10...30 % of 0.5...2.5 μm pores oriented in the direction of film growth were obtained by EBPVD on titanium, steel and stainless steel substrates. It was found that the morphology of pores can be controlled in accordance with specific needs by varying the condensation temperature $T_c = 0.4 \dots 0.55 \cdot T_{\text{Ti melt}}$ and the amount of NaCl. Such films are actually a metal frame with a developed system of micropores. They can be used both as an independent material and as a basis for the deposition of biocompatible materials, including $\text{Ca}_3(\text{PO}_4)_2$.

Fig. shows a composite multilayer material deposited during one technological cycle, which consists of 20 μm Ti layer and 75 μm porous Ti layer, coated with 12 μm $\text{Ca}_3(\text{PO}_4)_2$. The resulting material retains the open porosity. It is permeable and can be used as a implant coating to replace body tissues that will easily grow into the free space of the pores, gradually filling it.

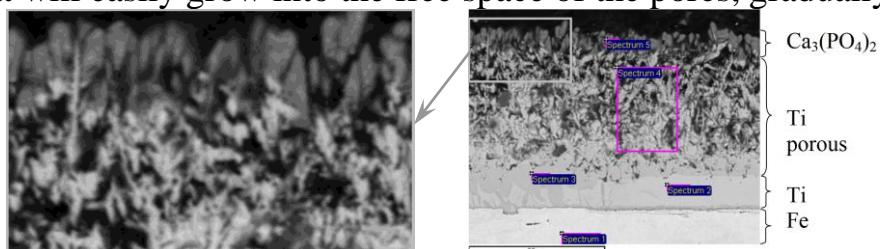


Fig. Multilayer composite material Ti - $\text{Ca}_3(\text{PO}_4)_2$

Specified porous Ti and composite Ti - $\text{Ca}_3(\text{PO}_4)_2$ films can also be modified with discrete nanoparticles or nanolayers of noble metals for obtainment of antiseptic (nano-Ag) or wound healing (nano-Au) characteristics. Discussed modification options can be applied technologically to surfaces of arbitrary shaped implants by EBPBD.

Influence of polyethylene morphology on the electrodynamic properties of segregated polymer composites with nanocarbon fillers

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It is known that an important parameter of quality of composite consisted of dielectric polymer and conductive nanocarbon filler is the filler dispersion in the polymer volume. The manufacture of so-called segregated composites allows the formation of an electrically conductive framework with a high local filler density and provides a uniform distribution of the filler in the volume of the composite sample. Depending on the method of manufacturing of segregated systems, there are different values of percolation transition φ_c , conductivity, the dielectric properties of CM, while φ_c does not depend on the type of polymer matrix and determined by the ratio of the sizes of the filler and the polymer particles, as well as the shape of the filler [1]. However, in our previous study we stated that the enhancement of electron transport properties in segregated composites is completely independent on the aspect ratios of fillers, but strongly depends on dielectric volume as well as on the type of spatial distribution of polymer particles [2]. The aim of this work is to investigate the influence of morphology of dielectric particles on the electrophysical characteristics of segregated polymer-nanocarbon structures. For this purpose, two different types of polyethylene powder were used as the polymer matrix: low-density polyethylene powder (high-pressure polyethylene) with a particle size of 0.1-0.3 mm and high molecular weight high-density polyethylene with a particle diameter of 100 μm . Graphite nanoplatelets, thermally exfoliated graphite, and multiwall carbon nanotubes were used as conductive fillers. The conductivity and electromagnetic response parameters of the fabricated composites were investigated. It is shown that the size distribution of polymer particles and their morphology play the same prominent role in improving the dielectric properties of the composite as the type and the morphology of the carbon filler.

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Regeneration of bentonite-coal sorbents after wastewater treatment

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For the sorption purification of process waste waters of industrial plants, many natural and synthetic materials are used. Activated carbon is used more often than others. Despite the intensive search for an alternative, no other material has been found yet that would be so effective as a sorbent.

Earlier, we have shown the possibility of obtaining hybrid bentonite-coal sorbents, based on bentonite clays and brown Angren coal [1].

With the obtained bentonite-coal sorbents, studies were carried out to purify and softening two samples of process water - circulating water and a tailing pond of the factory in Uzbekistan. This process water has a high hardness of more than 29 mg/eq.%. Heavy metal ions, sulfate ions, chlorides, cyanide and thiocyanide residues are found in its composition. Experiments were performed on 24 cleaning parameters. Natural sorbents were also used for comparison. After the treatment of these process water samples, bentonite-coal sorbents demonstrated activity in 18 parameters. Checking for water purity showed the absence of toxic compounds in the form of cyanide- (CN^-) and thiocyanide- (SCN^-) ions, heavy metal ions - chromium, nickel, beryllium *etc.* After wastewater treatment, the sorbents were regenerated. Taking into account the possibility of rapid sorbents destruction after thermal regeneration, the sorbents were chemically regenerated. 3 % sulfuric acid (H_2SO_4) and 3 % hydrogen peroxide (H_2O_2) were used as regenerates. After that, the sorbents were again used for wastewater treatment and the experiments on 24 cleaning parameters were performed repeatedly. It was revealed that the regeneration with sulfuric acid turned out to be better than with hydrogen peroxide. Of the 24 parameters studied, after regeneration with sulfuric acid, 22 parameters were restored, and after regeneration with hydrogen peroxide - 20 ones.

Thus, a single regeneration with strong oxidants showed positive results, which gives reason to assume the possibility of multiple regeneration of sorbents with subsequent determination of the strength degree of the bentonite-coal sorbents.

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Absorption of vitamins B1 and B3 on activated carbons from individual solutions and their mixtures

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Selective adsorption from the mixture is of particular interest in the extraction of useful components or for removing excess substances. Carbon adsorbents are widely used in the food industry to correct the smell, taste, colour and quality of food: stabilization of the colour, taste and smell of alcoholic beverages and juices caused by complex compounds such as polyphenols, melanoidin, anthocyanidins *etc.*; removal of molasses compounds from citric acid, lactic acid and other foodstuffs produced by biochemical processes; manufacture of many starch-based sweeteners, such as glucose, maltose, fructose, dextrose, *etc.* used in the production of soft drinks; removal of polycyclic aromatic hydrocarbons, polychlorinated biphenols, dioxins from vegetable oils; refining sugar and oils. For all these processes adsorbents with selective adsorption properties are used to minimize the removal of useful components and to extract unwanted components from the mixture.

This study presents the results obtained in modelling the adsorption processes of molecules of biogenic origin with different molecular weight on activated carbon AC-C (obtained from apricot kernels) and oenological activated carbon Granucol FA from individual solutions and their binary mixtures. Vitamins B1 ($M = 265.4 \text{ g/mol}$) and B3 ($M = 123.1 \text{ g/mol}$) were used as model molecules. The adsorption kinetics and isotherms of vitamins B1 and B3 from individual solutions were measured at three temperatures: 25, 35 and 45 °C. The study of the adsorption of vitamins B1 and B3 from equimolar binary mixtures on AC-C activated carbon showed that at low concentrations there is no selectivity to the studied substances, but with the increase of the initial concentration, vitamin B3 is mainly absorbed, the adsorption ratio reaching 28 and 72 % for vitamin B1 and B3 respectively. On Granucol FA activated carbon, the adsorption selectivity of vitamins B1 and B3 is 60 and 40 % at low concentrations, but with the increase of the initial concentration the adsorption selectivity decreases, and then the dependence becomes inverse.

Acknowledgements. This research was carried out with the financial support of the institutional project “The reduction of the environmental and health impact of toxic chemicals through use of adsorbents and catalysts obtained from local raw material” DISTOX, No 20.80009.7007.21.

The theoretical description for hydroxyquinol CoO(OH)-assisted electrochemical determination

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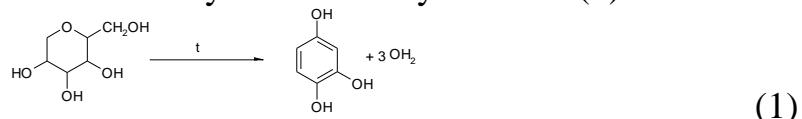
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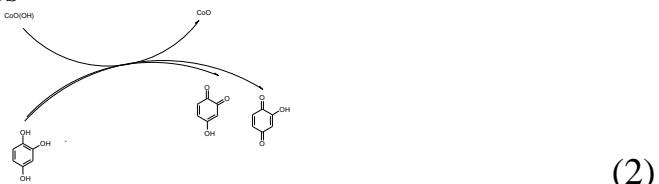
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Hydroxyquinol is one of the natural polyphenolic compounds, widely used as biomarkers and monomers for conducting polymers. Its natural occurrence is abundant and it is formed by fructose dehydratation (1):



On the other hand, hydroxyquinol is also a pharmaceutical wastewater pollutant, like its isomers, as it may be toxic for aquatic organisms. Therefore, the development of an efficient method for its quantification is really actual.

In this work, the electroanalytical process of the hydroxyquinol electrochemical determination, assisted by CoO(OH)-modified anode is theoretically analyzed by means of linear stability theory and bifurcation analysis. The electroanalytical process



is thereby described by a bivariant balance differential equation-set, and its analysis confirms that cobalt(III) oxyhydroxide may provide the precise and rapid hydroxyquinol electrochemical determination by a diffusion-controlled electroanalytical process.

Structural peculiarities, thermal and viscoelastic properties of ionomeric polyurethanes based on renewable raw materials

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A comprehensive solution to the environmental protection encourages looking for new ways to create environmentally friendly biodegradable polymeric materials by replacing the non-renewable components with biological ones. The work discusses the effect of naturally renewable components (castor (CO), palm (PO) oils, and xanthan (Xa)) on the structure, thermal and viscoelastic properties of nanosized aqueous anionic polyurethanes (APU). The structure-properties relationship was confirmed by WAXS, SAXS, DMA, TGA, and DSC analysis. The mass fraction of natural components in synthesized APU amounts to 70 %. It was shown that APUs with CO/PO content of 45 wt.%, (APU/CO₄₅), (APU/PO₄₅) as well as Xa-comprising polyurethanes (APU/CO₄₅/Xa₂₅) and (APU/PO₄₅/Xa₂₅) have, on the one hand, an amorphous structure, and on the other, a microphase structure. The type of oil affects the phase morphology and level of the structural heterogeneity of APU. PO-based polyurethanes are characterized by a higher level of structural heterogeneity. Xa dramatically changes the phase morphology and viscoelastic behaviour for both oil-comprising APUs. This results in significant decrease in tanδ and increase in E', which is caused by blocking of segmental mobility in both flexible and hard blocks due to the increase of intermolecular interaction between the polar groups of oil-containing APU and OH-groups of Xa. A pronounced glass transition (GT) is observed in the low-temperature region for APU, APU/CO₄₅, and APU/CO₄₅/Xa₂₅ (-68.5, -55.8 and -52.9 °C, respectively). However, the clearly pronounced GT disappears in APU/PO₄₅ and APU/PO₄₅/Xa₂₅ and an extended region appear in its place (-75÷0 °C), with distinguished weakly pronounced GT region at -62 °C and a GT-like extended region at -28 °C. The thermal stability of APU/CO₄₅ in the first stage of decomposition, vs APU and APU/PO₄₅ increases. Xa increases the rate of thermal decomposition in both oil-based APUs vs APU. Alternately in the high-temperature range (>400 °C), both oil-based APUs exhibit higher thermal stability vs APU. Thus, the increased content and nature of renewable raw materials allow control of their properties, structure, and degradation processes. Such polyurethanes can be used as polymer-carriers of biologically active substances in medicine, degradable packaging materials, as water-based adhesives, etc.

MCM-41 silicas with oligosaccharide “host” cavities for binding aromatic “guests”

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Amongst the numerous techniques for pollutant removal from aqueous solutions liquid-solid adsorption is the most widely used and favourable due to its high efficiency, easy practicality, and economic feasibility. Despite the large number of existing sorbents for water treatment, today there is a need to develop new types of materials with improved performance. Cyclodextrin-based silica materials usually display strong binding affinities for different water pollutants thanks to high adsorption capability of silica matrix with large surface area, high porosity, and excellent physicochemical properties as well as the ability of cyclodextrin moieties on the surface to form inclusion complexes “host”–“guest” type with various compounds [1].

In this work, mesoporous silica materials containing microporous cavities provided by covalent-bound β -cyclodextrin were synthesized by co-condensation of new type β -cyclodextrin-functionalized silane with tetraethyl orthosilicate using cetyltrimethylammonium bromide as structure directing agent. Several MCM-41 silicas with various degree of modification were prepared. Obtained materials were characterized by quantitative chemical analysis of surface compounds, IR spectroscopy, thermogravimetric analysis, X-ray diffraction, electron microscopy, low-temperature adsorption-desorption of nitrogen, and dynamic light scattering. The sorption of benzene and phenol on synthesized MCM-41 silicas from aqueous solution was studied as a function of time and equilibrium concentration. The experimental data were evaluated using typical kinetic and isotherm adsorption models. The probability of β -cyclodextrin-functionalized MCM-41 silicas use in water treatment processes was discussed.

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New zeolite anionic nanomaterial - preparation and properties

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Zeolites belong to the group of cation exchangers, so enriching them with potassium, ammonium or other cations is not difficult. This process is complicated by the presence of anions present in the corresponding compounds as anionic acid salts. When making anionic forms, zeolites should show high resemblance to ionic compounds. With such as salts, they should be easily occluded in this system. Salt cations and anions should be placed in the intracrystalline structure of zeolite in such a way as to avoid excessive collision of similarly charged ions. The role that the zeolite structure plays in this process is primarily related to the fact that zeolite is also a solid electrolyte and not just symmetrically arranged ordered pores and channels. A nanotechnological method for obtaining anion substituents is proposed, which is based on the introduction of the corresponding desired salt into the zeolite structure so that the obtained material does not lose its zeolite structure and acquires anion-exchange properties upon the formation of a new phase.

A certain amount of ammonium dihydrophosphate ($\text{NH}_4\text{H}_2\text{PO}_4$), potassium nitrate (KNO_3) and mixed cations (Fe, Ca, Mn, Mg, Zn, Cu, Mo, Co, Sn) were introduced into the nanoparticle by impregnation with in the structure of zeolite - clinoptilolite. Ammonium, nitrate and phosphate ions were detected in the zeolite nanomaterials treated with the corresponding salts, as well as the study of the zeolite structure by chemical analysis, IR spectroscopy and X-ray diffraction methods.

Acknowledgements

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Obtaining of new bactericidal zeolite fillers for papermaking

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In modern conditions, scientific research of various fillers is dynamically developing, providing improved characteristics of paper used as packaging material for transportation and storage of agricultural products, as well as food and industrial goods. The aim of our research is chemical modification of zeolite of Georgian origin, clinoptilolite-containing rock from the Rkoni plot of Tedzami deposit (Kaspi region, Eastern Georgia).

We have studied physical and chemical properties of clinoptilolite, to determine feasibility of application of white color natural clinoptilolite in paper industry as a filler. The solid-phase ion exchange method was used to obtain samples containing bioactive metals such as silver, copper and zinc.

Clinoptilolite is characterized by a three-dimensional structure of wide channels, which explains the high degree of substitution of natural compensating cations by transition metal ions; the rate of release of ions from zeolites decreases in the series $\text{Ag}^+ > \text{Zn}^{2+} \sim \text{Cu}^{2+}$. The samples obtained show bacteriostatic activity against *E. coli* and other pathogenic microorganisms.

According to the changes in the relative number of viable cells of bacteria contacting with zeolites and the data on leaching of metals from modified zeolites compared to the minimal inhibitory concentration (MIC) values for corresponding ions toward *E. coli*, the silver-containing zeolite exhibits a certain antibacterial activity even before the concentration of ions in the solution reaches the MIC value, and its bactericidal effect could be ascribed not only to released Ag^+ ions but also to Ag-zeolite itself; the copper- and zinc-containing zeolites emit a small amount of ions (up to 0.6 MIC) and their activity is entirely attributed to Cu-zeolite and Zn-zeolite themselves. Strong bacteriostatic activity of modified zeolites was established by the Kirby-Bauer test.

Identity of experimental and reference samples is confirmed by the preservation of the zeolite structure (XRD, FTIR, adsorption properties), enabling us to recommend clinoptilolite as a filler in the technology of manufacture of packing paper for foodstuff, since the raw material complies with European safety requirements.

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Low energy Electron Energy Loss Spectroscopy of the amorphous ribbon surface

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Low energy Electron Energy Loss Spectroscopy (EELS) has been employed for investigation of the electronic states of amorphous and crystalline $\text{Fe}_{73.6}\text{Cu}_{1}\text{Nb}_{2.4}\text{Si}_{15.8}\text{B}_{7.2}$ alloy surface and alloy components. This amorphous alloy with a nanocrystalline grain structure, known as FINEMET, is a very attractive soft magnetic material since it exhibits excellent permeability even in a high frequency range. Such a type of materials is prepared from a melt-spun amorphous material by annealing at temperatures higher than the crystallization temperature. Usually, FINEMET consists of ultra-fine grains of size a few nanometers, which has been thought to cause the soft magnetic properties. EELS is used to obtain physical-chemical state information as a function of the probing depth by varying the primary electron beam energy E_0 . EELS is very sensitive to the chemical state, and the atomic and electronic structure of the near surface region of the solid. Generally, EELS data relate to the characteristic electron losses which occur due to interband and intraband electronic transitions, ionization losses and surface and bulk plasmons.

Amorphous ribbons, about 25 μm thick and 10 mm wide, were prepared by a single-wheel melt-spinning technique. EELS peak-to-peak amplitude of the differentiated signal was obtained with a lock-in amplifier with 1-2 V modulation voltage. The energy resolution of the analyzer was $\Delta E/E = 0.1\text{-}0.3\%$ for energies $E_0 < 650 \text{ eV}$ The EEL spectra for the pure alloy components: Fe, the amorphised Si wafer, B, Nb, Cu and amorphous $\text{Fe}_{81}\text{B}_7\text{Si}_1\text{P}_{10}\text{Cu}_1$ alloy (free surface) for the primary electron beam energies E_0 ranging from 150 to 650 eV were measured. In the EELS spectra, we selected the following types of characteristic losses: interband and intraband transitions, surface (E_s) and bulk (E_b) plasmon, excitations and their hybrid modes. The following values of the plasmon energy for amorphous alloy were obtained (eV): $E_s = 15.2$; $E_b = 24.2$. It was shown that for the amorphous alloy the measured spectra have a complicated structure, but are similar to the spectra of Fe. The measured energies for the plasmon excitations were found not to agree with calculated values according to the classical theory for the collective oscillations in solids. for all specimens changes in the intensity energy E_s and E_b were observed depending on primary electron energy. With an increase in the energy of the primary electrons, a decrease and an increase in the intensity of the surface and bulk plasmons is observed, respectively.

Kinetic regularities of the impact of macrocyclic compound calix[4]arene C-956 on plasma membrane calcium pump and Ca²⁺ concentration in unexcited cells of the myometrium

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Plasma membrane (PM) Ca²⁺,Mg²⁺-ATPase maintains low calcium ions concentration in unexcited myocytes and leads to a decrease of Ca²⁺ concentration in myoplasm after muscle contraction. Accordingly, the search for a compound that would alter the activity of PM Ca²⁺-pump is promising. From this point of view, the calixarenes are very interesting and perspective compounds, because we showed in previous experiments that calix[4]arene C-956 selectively (relative to other ATP-hydrolases of PM) inhibit the activity of Ca²⁺,Mg²⁺-ATPase ($I_{0,5} = 15.0 \pm 0.5 \mu\text{M}$).

Thus, the aim of this work was to study the dependence of kinetic parameters of calix[4]arene C-956 inhibition of PM Ca²⁺,Mg²⁺-ATPase on the concentration of Mg, Ca and ATP ions. Calix[4]arenes were synthesized by academician of the NASU V.I. Kalchenko and his colleagues in the Phosphoranes Chemistry Department of the Institute of Organic Chemistry, NASU. Experiments were performed on the PM fraction processed by 0.1 % digitonin, and suspension of myometrium cells.

We studied the dependence of PM Ca²⁺,Mg²⁺-ATPase specific activity on the concentration of Mg, Ca and ATP ions in incubation medium at different calix[4]arene C-956 concentrations (1, 10, 30, 60 and 100 μM , respectively). We demonstrated that calix[4]arene C-956 do not affect the activation constants by Ca and Mg ions, and Michaelis constant K_m by ATP, but this compound decreases the maximum initial rate V_{\max} of ATP hydrolysis reaction in all cases. Thus, calix[4]arene C-956 acts as a complete non-competitive inhibitor of PM Ca²⁺,Mg²⁺-ATPase.

Using confocal microscopy we showed that this compound increases Ca²⁺ concentration in myometrium cells.

The obtained data can provide the basis for using of calix[4]arene C-956 as a selective and effective inhibitor of PM Ca²⁺,Mg²⁺-ATPase that can be important for further investigation of the membrane mechanisms of Ca²⁺ exchange in the smooth muscles, in particular, PM participation in electromechanical coupling in smooth muscles.

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Nanocomposite surgical suture materials, allografts for tissue joining and tissue alloplastic

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The problem of tissue joining and tissue alloplastic remains one of the most pressing problems of modern surgery. By modifying polypropylene with carbon nanotubes, silver nanoparticles and antiseptics, new types of surgical suture materials and allografts for tissue plastics had been developed.

Purpose of the study was to substantiate the efficiency of using nanocomposite surgical suture materials and allografts with antimicrobial properties for tissue joining and tissue alloplastic.

The investigation of the developed materials properties and allografts the study of their physicochemical, mechanical, antimicrobial and manipulative properties and the possibility of sterilization by different methods were included. In the experiment had been studied the biocompatibility of the developed materials with tissues, followed by testing the effectiveness of their use in the clinic as surgical suture material and allografts for tissue plastics in the treatment of abdominal hernias. The obtained digital data after statistical processing was compared with the data obtained in the study of known materials.

Studies had shown that the introduction of nanocomposites and antiseptics into polypropylene made it possible to obtain new surgical suture materials, which were superior in their properties to the known ones. The developed threads had high strength, no wicking and capillarity, good handling properties, antimicrobial activity, did not lose their properties during sterilization, and had high biocompatibility with tissues. The use of the developed suture materials in the clinic showed high efficiency of tissue joining. The results obtained in the study of the developed threads properties served as the basis for the creation of new types of mesh allografts for tissue plastics, which had a number of advantages over the known mesh allografts made of polypropylene. Experimental studies had shown that after its implantation around the implants, a moderate inflammatory reaction of tissues arose, a thin connective tissue capsule was quickly formed and antimicrobial activity persisted for a long time. Positive results of using in the clinic developed allografts have indicated on the future prospects of using such materials for the prevention of postoperative complications were obtained.

The place of nanodispersed silica in the treatment of endogenous intoxication in patients with COVID-19 associated pneumonia: New approaches

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One of the biggest challenges in the modern medical world is endogenous intoxication (EI) in patients with community-acquired pneumonia (CAP) caused by SARS-CoV-2. Despite the active search for and continuous improvement of modern tactic of this disease treatment, mortality is at a very high level, which requires new approaches to treatment. We have developed a method of treating COVID-19-associated CAP, which includes a traditional treatment regimen and enterosorption of nanodispersed silica.

Purpose of investigation is to evaluate the effectiveness of efferent therapy based on silica nanoparticles in the treatment of COVID-19-associated CAP.

The study was performed in 82 patients with CAP and COVID-19. They were divided into two groups: main (42 patients) and comparative (40 patients) groups, which were representative by age and sex. In the comparison group, patients received treatment according to the existing protocol, and in the study group additionally performed efferent therapy with nanodispersed silica. Evaluation of the effectiveness of the developed method was performed with using clinical, laboratory methods and determination of the EI level.

Studies have shown that patients in the main group had faster ($p \leq 0.05$) normalization of all EI parameters, which indicated a more favorable course of the disease. Complications in this group were significantly ($p \leq 0.05$) lower than in the comparison group. Treatment of patients with CAP and COVID-19 with efferent therapy showed a significant ($p \leq 0.05$) reduction in duration of hospitalization, reduction in complications and mortality.

The use of nanodispersed silica to reduce EI in patients with CAP and COVID-19 may significantly improve the outcomes of this pathology treatment, which requires further study.

Perspectives of the usage of nano-antioxidants for cardiovascular diseases therapy

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Cardiovascular disease (CVD) remains the greatest killer in the World. Ischemia/reperfusion injury (IRI) is the pathological condition that occurs at CVD caused by reactive oxygen species (ROS) [1]. Besides such CVD as atherosclerosis, ischemic heart disease, hypertension, cardiomyopathy, etc., ROS-mediated oxidative stress is also implicated in diabetes, carcinogenesis and neurodegeneration, autoimmune diseases, alcoholic liver disease, and various inflammation-related disorders [2].

Recently, it was found that nanomaterials can mimic the properties of antioxidant enzymes to inhibit apoptosis and improve the cell survival after IRI [3]. Unique physicochemical properties of materials at the nanolevel such as large surface-to-volume ratio, surface chemistry, and the possibility of targeted delivery to desired tissues make them good candidates for biomedical applications. Among them, metal oxides nanoparticles, noble metal materials, metal halides, hybrid materials have been found to possess an intrinsic enzyme-mimetic activity [4-7]. Carbon-based nanomaterials may also show ROS scavenging effects [8]. All carbon-based materials showed significant performance against OH* radical, modest activity against hydrogen peroxide and lipid peroxy radicals and stable radicals including DPPH and ABTS, specially graphene oxide [9]. Considering Gr as antioxidants for using *in vivo*, a set of questions remain unclear, specially its biocompatibility. Nevertheless, the first attempts showed the good perspective of using of graphene for CVD.

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Technology of creating ceramic materials based on the system $\text{BaO} - \text{SrO} - \text{Al}_2\text{O}_3 - \text{SiO}_2$

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Nowadays, the creation of radio-transparent ceramic materials with a set of high performance characteristics and improvement of technological parameters for the manufacture of parts of complex shapes with different sizes is an urgent need of the modern aerospace industry.

To develop the technology of creating products from radio-transparent ceramics, in particular the stage of forming samples, the method of casting water slips was studied. At the previous stage of research, the composition of the ceramic mass was obtained on the basis of the phases of Celsian and Slavsonite, which are part of the system $\text{BaO} - \text{SrO} - \text{Al}_2\text{O}_3 - \text{SiO}_2$ ($\text{SiO}_2 - 31.26$; $\text{Al}_2\text{O}_3 - 26.58$; $\text{BaO} - 9.01$; $\text{SrO} - 20.95$; $\text{Fe}_2\text{O}_3 - 0.02$; $\text{CaO} - 0.01$; $\text{Na}_2\text{O} - 0.07$) and the optimal intensifying additive for their sintering ($\text{Li}_2\text{O} - 0.18$; $\text{SnO} - 0.59$). As raw materials used quartz (silicon oxide (IV) (hd)), alumina grade Г-00 (aluminum oxide (hd)), barium carbonate (hd), strontium carbonate (hd), lithium carbonate and tin oxide.

Using the method of mathematical planning (PFE 2³), it was found that in the study area of technological parameters of the best properties of the material acquires a content of 0.1 wt.% of Dolapix PC 67 additive, 30 minutes of grinding and at a firing temperature of 1350 °C. The created material is characterized by the following indicators: water absorption - 0.07 %, apparent density - 3.06 g/cm³ and flexural strength - 72.50 MPa.

The results of qualitative X-ray phase analysis and electron microscopy showed that at firing temperatures above 1250 °C in all samples there is only the phase $\text{Ba}_{0.25}\text{Sr}_{0.75}\text{Al}_2\text{Si}_2\text{O}_8$, and the structure of ceramic samples is represented by barium strontium anortite is homogeneous, without defects and cracks.

According to the results of complex research, the following technological parameters of production are recommended: firing at the stage of synthesis at a temperature of 1200 °C with a 2-hour exposure; grinding the synthesis products in a ball mill to ensure a residue on the sieve № 0063 not more than 1 % with the addition of 0.1 wt.% of Dolapix PS 67 additive and slip moisture content – 30 %. Casting of blanks from slip into gypsum forms; firing of products at a temperature of 1350 °C with 2 hours endurance.

Study of the influence of ferromagnetic additives on composite ceramics

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To create materials and coatings that effectively protect in the ultrahigh frequency range, it is necessary to use ferrites that have low values of magnetic permeability at low frequencies. On the basis of magnetic materials, thin composite coatings are obtained, so magnetic additives are better used in watering, because they form a thin layer.

As magnetic additives in ceramic materials are mainly used metals, their alloys (iron carbonyl, magnetite, iron-nickel alloy) and ferrites (manganese-zinc, nickel-zinc, magnesium, nickel, cobalt, zinc, copper). Given the requirements for these additives, cobalt ferrites (CoFe_2O_4), copper (CuFe_2O_4) and zinc (ZnFe_2O_4) were selected for research.

Ferrites were synthesized in a laboratory silite furnace at a temperature of 1150 °C, the duration of firing at maximum temperature was 8 hours. To study the effect of these additives on glass crystalline irrigation, alkali-free boron-containing glass composition was chosen as the basis. A cathode oscilloscope was used to determine the magnetic characteristics of the obtained materials.

It is established that only cobalt ferrite has magnetic properties (maximum value of magnetic permeability is 252). The effect of CoFe_2O_4 additive on glass crystal irrigation with the ratio of $\text{CoO} : \text{Fe}_2\text{O}_3$ oxides from 1:0.6 to 1:5.2 was studied. Chemical composition of watering, wt.%: $\text{SiO}_2 - 45$; $\text{Al}_2\text{O}_3 - 7$; $\text{B}_2\text{O}_3 - 10$; $\text{MgO} - 3$; $\text{CaO} - 7$; $\text{CoO} - 7$; $\text{Fe}_2\text{O}_3 - 21$. It was found that when adding 30 % of the additive in the ratio $\text{CoO} : \text{Fe}_2\text{O}_3$ 1:1.5 irrigation was characterized by the following properties: magnetic permeability - 7.28; dielectric constant (at frequencies of 10 - 100 kHz) - 6.78 - 7.26; the tangent of the dielectric loss angle (at frequencies of 10 - 100 kHz) - 0.065 – 0.188; specific volume resistance - $0.49 \cdot 10^6 \text{ Om m}$; density - 4190 kg/m^3 ; temperature coefficient of linear expansion – $3.789 \cdot 10^6 \text{ deg}^{-1}$.

From this we can conclude that using the ferrite CoFe_2O_4 as a special additive to create a coating on a ceramic composite material, you can get a magnetic coating that protects against electromagnetic radiation, which will weaken the electromagnetic energy due to energy losses on reversal and vortex losses currents. Further research is aimed at studying the magnetic properties in the region of ultrahigh frequencies.

Influence of copper nanoparticles on the electrosurface and biochemical parameters of bacterial cells

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The colloidal form of copper is perspective for development of new medicinal preparations. The copper nanoparticles (CuNPs) of determined size and concentration range are able to demonstrate both stimulation and inhibition of biological activity. Impact research of CuNPs on the functional state of bacterial cells gives an opportunity to control and regulate the intensity of their physiological and biochemical reactions. Data obtained can be useful for development of metal-containing preparations of probiotics and vaccines for a prophylaxis and treatment of various diseases of man and animals.

This work presents the experimental results on study of electrosurface, electrochemical and biochemical parameters change of *B. cereus* B4368 cells in reply to the action of CuNPs as compared to their ionic form. The nanoparticles used were synthesized from copper sulfate solution with NaBH₄ in the presence of PEG. The average size of the particles presented was about 20 nm. The results obtained demonstrated a decrease of cells negative ζ -potential (-38 mV) by 74 % after their contact with copper nanoparticles against 16 % in the case of ionic metal form at the same dose. This testifies to effective concentration dependent CuNPs heterocoagulation with bacterial cells as well as Cu²⁺ ions sorption. Note that, the synthesized CuNPs in a solution environment with low acid and close to neutral pH value carried on the surface positive charge due to presence at their surface thin copper oxide layer and its solubility. Membrane ATPase, which is the main transmembrane potential generator of bacterial cells, reacted on the contact with copper preparations by inhibition of its activity. Inhibition level of ATPase activity by CuNPs turned out to be on average 20 % higher as the same rate for anionic form. The transmembrane potential level showed the dissipation value about 52 % under CuNPs treatment against 35 % for Cu²⁺. In concentration range 15÷100 μ M, the toxic copper influence is more pronounced for its colloidal form with the most significant increase at low acid and neutral pH value. This correlates with the effect of the ionic and colloidal copper forms on ζ - potential value. It takes place the effective accumulation of positive charged CuNPs on a cell surface. Nanoparticles may serve as a reservoir of active Cu²⁺-ions, which interact with biochemical structures. In addition, the violation of barrier function of plasmatic membrane is also possible.

Composite materials based on TiO₂ and activated carbon for elimination and photodegradation of adsorbable organic halogens

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Adsorbable organohalogens are persistent organic pollutants frequently found in water, which pose serious environmental and health issues. Their degradation and/or removal become an important challenge. Among the existing technologies of removal and treatment of different pollutants, photodegradation using semiconductor catalyst is a promising alternative method [1]. Nonetheless, the typical weak adsorption capacity of this photocatalyst is an issue for the degradation process. To overcome this limitation, photocatalyst/adsorbent composites based on high surface area activated carbons and TiO₂ can be used [2]. TiO₂ supported activated carbon shows synergistic effect in organic pollutants removal due to the enhancing the lifetime of electron-hole pair and the rate of hydroxyl radical production caused by presence of activated carbon background.

The present study deals with facile *in situ* sol-gel synthesis of composite material based on TiO₂ and granular activated carbon. SEM-EDX analysis showed that TiO₂ was unevenly distributed on carrier's surface. The synthesized composite has the high surface area (907 m²/g) and relatively high content of crystalline phase (21.9 %). According to Rietveld refinement, the composition of crystalline part is 66.6 % anatase, 7.1 % rutile and 26.3 % of titanates. IR investigations revealed that TiO₂ was connected to the carrier's surface, probably, by means of H-bonds between NH₂- groups on GAC surface and OH-surface groups of TiO₂. The adsorption experiments indicated high adsorption capacity of synthesized composite towards 4-halogenphenols as the model AOX substances. Therefore, such benefits allow its application for adsorption and/or degradation of organic pollutants.

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Electronic structure of bulk metallic glasses based on iron

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Bulk metallic glasses (BMGs) are a new class of amorphous metal alloys (AMA) with improved physical properties, the ability to modify their structure, and the ability to form in a state of supercooled liquid, which provides much greater opportunities for their use compared to conventional AMA.

To date, there is no definitive model for the predicted synthesis of BMGs with specified characteristics, so the study of the structure and physicochemical properties of the first synthesized compounds is a necessary basis for creating such a model.

The peculiarities of the electronic structure of iron-based complex-alloyed BMG have been studied by the XPS method ($\text{Fe}_{55}\text{Ni}_8\text{Co}_6\text{Mo}_4\text{Cr}_2\text{V}_1\text{Al}_2\text{P}_9\text{C}_6\text{B}_5\text{Si}_2$ and $\text{Fe}_{61.37}\text{Cr}_{3.78}\text{Co}_{6.84}\text{V}_{0.82}\text{Mo}_{1.06}\text{Nb}_{0.85}\text{B}_{19.87}\text{C}_{1.99}\text{Si}_{2.57}$).

Established the presence of a significant oxidized layer at the depth up to 150 nm, while deep in the volume, the oxygen concentration is significantly lower.

In the volume of the studied samples, carbon is mainly found in compounds with boron and iron (while on the surface - with oxygen), and the presence of iron carbide and boride is detected.

Analysis of the bonds according to the XPS shows that the Co and Si (in the case of $\text{Fe}_{61.37}\text{Cr}_{3.78}\text{Co}_{6.84}\text{V}_{0.82}\text{Mo}_{1.06}\text{Nb}_{0.85}\text{B}_{19.87}\text{C}_{1.99}\text{Si}_{2.57}$) and Ni, Co, Mo, Al, Si (in the case of $\text{Fe}_{55}\text{Ni}_8\text{Co}_6\text{Mo}_4\text{Cr}_2\text{V}_1\text{Al}_2\text{P}_9\text{C}_6\text{B}_5\text{Si}_2$) are mainly found in the oxygen matrix, which eliminates the bond with iron carbides and borides.

It has been shown that the concentration of boron in BMGs plays a significant role in the formation of carbon bonds with metallic components.

Given that the distance Fe Me (where Me = Ni, Co, Mo, Al or Si) is close to the distance between the iron atoms and exceeds the length of the bond of iron with boron, the atoms of Ni, Co, Mo, Al and Si in the formation of nanosized crystal structures occupy Fe positions due to diffusion, which is one of the possible mechanisms of surface segregation.

Electrochemical impedance spectroscopy as a method to predict and improve the supercapacitor performance

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Supercapacitors (SC) are energy storage devices comprising two nanocarbon electrodes applied on current collectors, separated by a porous insulating film (separator) and immersed in a liquid electrolyte [1]. The energy stored in SC depends mostly on the electrode pore structure and surface area accessible for the electrolyte to form the electric double layer. The SC internal resistance and, hence, their power capability and efficiency, depend on the conductivity of electrode components and electrolyte, on the slowdown of ion diffusion in nanopores and on the electrode fabrication technique. Various electrochemical methods are used to measure the key SC characteristics, such as capacitance and internal resistance. The commonly used are cyclic voltammetry (CV) and galvanostatic charge-discharge cycling, which are time consuming and may affect the device characteristics. Electrochemical impedance spectroscopy (EIS) is another technique that can provide both capacitance and resistance values at various voltages and with a negligible influence on the system.

In this work the main attention is paid to SC impedance spectra and how they can be interpreted for electrode material characterization according to the equivalent circuit chosen. All the elements or blocks in the equivalent circuit model describe the corresponding physical processes occurring in SC and can be used to predict and improve the SC performance.

In this work EIS spectra for four type of commercially available active carbons and two graphene-type materials were studied. In particular, the attention was paid to pros and cons of these materials to be used in SC electrodes. Three major ranges of the EIS spectra were thoroughly investigated. The low frequency range gave us a chance to evaluate a boundary value of capacitance [2], while in the high frequency range the internal resistance was measured [3]. Medium frequency range allowed us to see whether a passive layer was formed at the current collector surface and to determine a contribution from different pore types into the total capacitance [4].

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Graft copolymer-assisted synthesis of nickel nanoparticles

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Nickel nanoparticles (NiNPs) have received increased attention in recent years due to their catalytic, magnetic, absorption, biocidal, anti-inflammatory and anti-cancer properties. The participation of polymers in the preparation and stabilization of NiNPs contributes to the control of the size, shape, crystallinity, oxidizability, magnetic and catalytic properties of these nanoparticles. In this context, a special graft copolymer with interacting poly(vinyl alcohol) backbone and polyacrylamide chains (PVA-g-PAAm) was synthesized, characterized and used as a matrix for the *in situ* synthesis of NiNPs in aqueous media.

Matrix solutions contained individual copolymer macromolecules (monomolecular micelles) of ellipsoidal shape and their fractal aggregates. To study the process of borohydride reduction of Ni²⁺-ions in PVA-g-PAAm solutions, an original method for monitoring the kinetics of the formation of metal nanoparticles was proposed and implemented for the cases where there is no surface plasmon resonance band in UV-Vis spectra. An increase in the initial rate of accumulation and yield of NiNPs with an increase in the concentration of Ni-salt and a decrease in both parameters in copolymer solutions in comparison with pure water were found. The complex role of matrix concentration has also been shown. In the final compositions NiNPs/PVA-g-PAAm, the emergence of new structures such as “hairy coils” and “hairy rods” with separate small spherical NiNPs and their chains was identified and explained (Fig.).

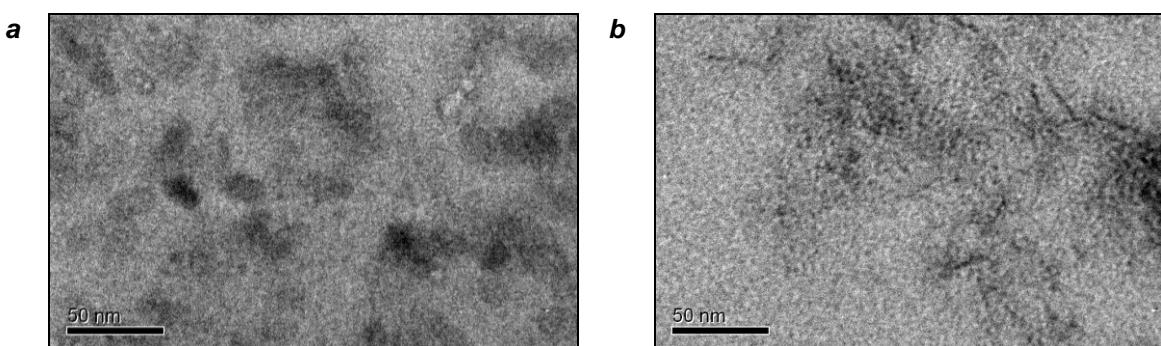


Fig. NiNPs/PVA-g-PAAm compositions containing predominantly (a) “hairy coils” and (b) “hairy rods” with small isolated and chain-linked NiNPs

Fractional advection-diffusion in a porous medium with fractal geometry

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In a porous fractal medium, the transport dynamics sometimes follows anomalous behavior [1]. Moreover, the crossovers between various transport regimes are observed [2].

In this study, we experimentally investigate the mass transfer of methane and methanol through the composite porous particle containing zeolite ZSM-5 and alumina. This porous material is found to be characterized by fractal geometry. It is shown that transport mechanisms differ at short and long times. At relatively short times, pure advection is observed. In contrast, the transport at medium and long times follows a convective mechanism. Depending on the diffusing agent, the longtime mass transfer obeys either Fickian or non-Fickian kinetics. Particularly, for methanol, which is characterized by higher adsorption energy, the anomalous transport is verified. Methane transport dynamics is usual Fickian, whereas its adsorption energy is considerably lower compared to methanol. The obtained findings allow us to speculate that non-Fickian transport arises due to the strong irreversible adsorption sticking of the diffusing molecules on the surface of the porous particle.

These results are obtained using the developed analytic solutions of the advection, advection-diffusion, and fractional advection-diffusion equations. For the distinguishing of the transport regimes, an approach admitting the transformations of the experimental data and the relevant analytic solutions in either semi-logarithmic or logarithmic coordinates is developed. The time-fractional advection-diffusion equation is used on a phenomenological basis to describe the experimental data exhibiting non-Fickian kinetics. The obtained anomalous diffusion exponent corresponds to the superdiffusive transport.

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Complex forming properties of anesthetics with transition metals

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Industry of pharmacological preparations is quite diverse. In the production of medicinal substances, coordination (chelate) compounds occupy a significant place. Complexes of the following composition have been synthesized: $\text{Me}(\text{Ans})_2\text{X}_2$ and $(\text{AnsH})_2[\text{MeX}_4]\cdot\text{nH}_2\text{O}$, where $\text{X}=\text{Cl}^-$, NCS^- ; Ans - lidocaine ($\text{Lid}\cdot\text{HCl}$), trimecaine ($\text{Tm}\cdot\text{HCl}$), anesthesin (ANS). The complex forming properties of Mn(II), Cu(II), Zn(II), Sn(II) salts and other biometals with anesthetic ligands was studied using IR spectra, thermoanalytical TG-DTG / DTA, spectrophotometry and single-crystal X-ray diffraction methods. Complex forming properties in the Fe(III) - Lid·HCl - NCS⁻ system was studied. The complex is extracted with ether, isobutyl alcohol and chloroform. The best extractant is chloroform, as it evaporates less. Extracts containing only Cu(II), Co(II) and Fe(III) ions are the only colored ones from the tested cations.

Among them, the most sensitive are Fe(III) complexes. Relevant X-ray diffractometric analysis details are set out here: 1) $(\text{LidH})_2[\text{ZnCl}_4]$ crystallizes in the monoclinic space group $P2_1/c$ with $a = 8.8921(2)$, $b = 19.2650(3)$, $c = 19.3211(3)$ Å, and $Z = 4$, $D_c = 1.366 \text{ Mg/m}^3$, and consists of the ZnCl_4^{2-} slightly distorted tetrahedral anion and two protonated cations of lidocaine LidH^+ in an outer coordination field; 2). $(\text{LidH})_2[\text{Ni}(\text{NCS})_4\cdot 2\text{H}_2\text{O}]$ crystallizes in the monoclinic space group $P2_1/c$ with $a = 18.3509(5)$, $b = 7.6532(2)$, $c = 14.9585(4)$ Å, $\beta = 109.964(2)^\circ$, $V = 1974.57(9)$ Å, and $Z=2$, forming structure of molecular crystal with slightly distorted $\text{Ni}[(\text{NCS})_4(\text{H}_2\text{O})]^{2-}$ octahedrons symmetrically associated with two LidH^+ ions by hydrogen bonds. 3). $(\text{TmH})_2[\text{SnX}_6]\cdot\text{H}_2\text{O}$ crystallizes in the rhombic space group $P2_12_12_1$ with $a = 10.745(1)$, $b = 14.199(2)$, $c = 26.166(3)$ Å, and $Z = 4$, forming structure of molecular crystal with distorted $[\text{SnX}_6]^{2-}$ octahedrons asymmetrically associated with water molecule and two TmH^+ ions by two $\text{Cl}\dots\text{HO}$, $\text{O}\dots\text{HN}$ and bifurcated $\text{NH}\dots\text{2Cl}$ hydrogen bonds. Polyhedrons of metal atoms in structures are distorted tetrahedron or octahedron.

The data obtained make it possible to judge the effect of the nature of the anion, the structure of the organic ligand, and the experimental conditions on the degree of complexing properties of the anesthetics studied in the work. The complexes are convenient model compounds for long-acting high-molecular-weight drugs.

Nano-structuring in the coatings prepared from CVD-composites

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CVD (Chemical Vapor Deposition) - composites are a new class of materials for interference optics in the IR spectral range based on germanium - metal chalcogenide (oxide) systems (ZnS, SbSe₃, GeO₂). Their feature is the practically congruent nature of evaporation in a vacuum, i.e. they behave like compounds. In contrast, CVD-composites have a higher volatility than individual components. At high temperatures and vacuum the starting components react with each other to form more volatile compounds. During condensation on a cold substrate the regeneration of components in the form of a nanostructured composite occurs. This is confirmed by XRPD: for example, if the diffractogram of the CVD-composite clearly shows peaks corresponding to its components, then the diffractogram of the coating is an unstructured curve with a "halo" in the whole range of Bragg angles (Fig.1). Perhaps this is due to the extremely high amorphization capacity of germanium itself in the thin-film state. In this case, the germanium coating exhibits a noticeably pronounced "blue" (gypsochromic) shift of the transmission region boundary in the short-wavelength range. Based on it, the size of germanium nanoparticles in the coating was estimated as 5.7 nm [1]. Using high-resolution transmission electron microscopy (TEM), the amorphous nature of the coating obtained by thermal evaporation in vacuum of the Ge-Sb₂Se₃ CVD composite was confirmed (Fig.2).

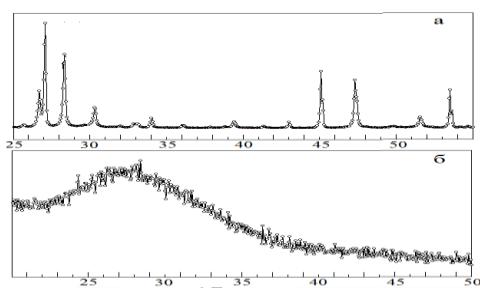


Fig.1. Patterns of diffraction spectra of a CVD-composite Ge-ZnS (a) and coating (b)

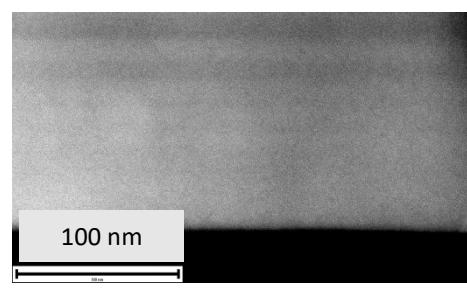


Fig.2. TEM of a CVD-composite Ge-Sb₂Se₃ coating on a glass substrate

1. V.F. Zinchenko, V.P. Sobol', O.V. Sviridova, Phys. Chem. Solid State. **13** (1) (2012) 197.

3D products from composites based on Al₂O₃ and carbon nanotubes using CJP 3D printing technology

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Carbon nanostructures (CNS) with high electrical conductivity, thermal conductivity, chemical and thermal stability, as well as high mechanical strength are currently of great interest for materials science.

One of the promising areas of materials science is the formation of various composites containing carbon nanotubes (CNTs) in order to increase their thermal and electrical conductivity, as well as strength and tribological characteristics.

Carbon-ceramic composites were obtained by mechanical mixing (in a planetary ball mill) powders of Al₂O₃ and CNTs in different weight proportions (1 %, 2 %, 3 %, 4 % and 5 % of the CNT mass), and by the synthesis of carbon nanotubes in the bulk of the Al₂O₃ powder, which ensured a more uniform distribution of the tubes in the bulk. Such carbon-ceramic composites are well suited for use in CJP 3D printing technology.

At a low CNT content (1-2wt.%) in the composite, the electrical conductivity practically does not change and is about 5×10^{-8} Ohm/cm. An increase in the content of nanotubes to 5° wt.% leads to a sharp increase in electrical conductivity up to 3×10^{-4} Ohm/cm.

Conclusions: Using the CJP 3D printing technology, a ceramic material was obtained, into which carbon nanotubes were introduced, which increased the electrical conductivity of Al₂O₃ by more than 4 orders of magnitude.

A sharp rise in the bending strength of the sintered specimen was also recorded, depending on the amount of CNTs in the composite.

Hydrogen solubility in Me(BC)_nH_x, where Me = Li, Na, Mg, Ca

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In recent years the hydrogen-sorption properties of magnesium-containing systems has been studied intensively since these compounds have been very promising for the hydrogen storage.

The statistical calculation of hydrogen sorption properties of compounds Me(BC)_nH_x (M=Li, Na, Mg, Ca, 0<x<12, n=1 and 2 for alkali and alkali-earth metals respectively) has been performed in the perspective that such hydroborocarbides will be the reliable materials for the reversible storage of hydrogen in large quantities. The calculation of free energy of crystal has been carried out, the equation of thermodynamic equilibrium of the system, which determines the *P-T-c* phase diagram, has been obtained.

The hydrogen solubility in borocarbides of these metals has been estimated in dependence on temperature and external pressure. The plots of these dependences have been constructed. The possibility of manifestation of hysteresis effect has been established. These formulae allow to establish the *P, T* conditions of high hydrogen content in these systems.

For known values of the energetic parameters of different metals borocarbides from independent experiments the derived equations permit to select the optimum composition of material and to develop the experimental technology for solving of the practical problems – to select the system, its composition and to ascertain the optimal *P, T* conditions of the reversible accumulation of hydrogen in this system.

Chemiluminescent reactions of heteropoly acids and their complexes with cationic surfactants in aqueous solutions and on the carriers surface

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Chemiluminescent (CL) reactions with luminol of heteropoly acids (HPA) $H_4PVMo_{11}O_{40}$, $H_4AsVMo_{11}O_{40}$, $H_4SiMo_{12}O_{40}$, $H_5GeVMo_{11}O_{40}$ in aqueous solutions, as well as after immobilization on cellulose and DEAE-cellulose filters, have been studied. A scheme of CL reactions was proposed, including catalytic oxidation of the luminol anion to the semiquinone radical by atmospheric oxygen through the HPA redox cycle, oxidation of the semiquinone radical with oxygen to form diazaquinone and superoxide radical anion, oxidation of the semiquinone radical by superoxide to luminol peroxide, which further decomposes to aminophthalate with light emission. Carrying out reactions with a luminol solution directly on the surface of the sorbent makes it possible to achieve high sensitivity for the determination of P, As, Ge, Si due to preconcentration of HPA during sample filtration.

The composition of poorly soluble ionic associates (IA) of the listed HPA with long-chain cationic surfactants (dodecylpyridinium bromide DDPB, tetradecylpyridinium bromide TDPB, cetyltrimethylammonium bromide CTB) was investigated by Bjerrum's method, by equilibrium shift method and by molar ratio method after filtration through cellulose filters using CL reactions of isolated IA with luminol. Integral light amount and maximum light intensity were used as characteristics of the system.

The composition of IA HPA-surfactant is determined: $(CT)_4SiMo_{12}O_{40}$; $(CT)_5GeVMo_{11}O_{40}$; $(TDP)_4AsVMo_{11}O_{40}$; in the case of molybdovanadophosphoric acid, the composition of IA is different at different pH: at pH 1.0, the composition of IA is $(DDP)_3H[PVMo_{11}O_{40}]$; at pH 1.7 – $(DDP)_4[PVMo_{11}O_{40}]$. This result is consistent with the data that the fourth proton in $H_4PVMo_{11}O_{40}$ is weakly dissociated; it is more strongly bound to HPA and is localized on the oxygen atom of the Mo–O–Mo angular bond. Thus, as a result of protonation of HPA upon going from pH 1.7 to pH 1.0, the acid $H_4PVMo_{11}O_{40}$ forms not tetra-substituted, but triply substituted IA.

IA HPA-cationic surfactant reacts with an alkaline solution of luminol with light emission similarly to HPA themselves. Their isolation on cellulose filters and detection by CL method directly on the sorbent surface made it possible to improve the sensitivity of the determination of P, As, Si, Ge 2–3 times.

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