

Ilia V. Chepkasov

Curriculum Vitae

PERSONAL DATA

Affiliation Senior Research Scientist, Skolkovo Institute of Science and Technology, Moscow, Russia
Date of birth October 5, 1988
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RESEARCH INTERESTS

nanoparticles, gas-phase condensation, electron properties of nanoalloy, catalytic properties of nanoalloy, 2D material, DFT, MD, machine learning interatomic potentials, thermoelectric materials, structure prediction.

OTHER SKILLS

Scientific programs: VMD, Ovito, Origin, VESTA, Python, LAMMPS, DL_POLY, OpenMX, VASP, QuantumATK, USPEX, Phonopy, Lobster, MLIP, AICON.

EMPLOYMENT and POSITIONS

08/2020 - present	Skolkovo Institute of Science and Technology, senior research scientist, Project Center for Energy Transition and ESG	Moscow, Russia
03/2021 -- 09/2021	Helmholtz-Zentrum Dresden-Rossendorf visiting researcher at the Atomistic simulations of irradiation-induced phenomena	Dresden, Germany
06/2019 - 08/2020	National University of Science and Technology "MISIS", visiting researcher at the Inorganic Nanomaterial Laboratory	Moscow, Russia
10/2018 - 03/2019	Helmholtz-Zentrum Dresden-Rossendorf visiting researcher at the Atomistic simulations of irradiation-induced phenomena	Dresden, Germany
1/2014 - 10/2018	Katanov Khakas State University researcher at the Nanophysics Laboratory	Abakan, Russia
6/2014 - 08/2020	Katanov Khakas State University assistant professor at the Department of Physics	Abakan, Russia
9/2012 - 12/2012	Institute of Metallurgy of the Ural Branch of the RAS junior researcher at the Group of RAS Advisor (Internship)	Ekaterinburg, Russia

EDUCATION and DEGREES

10/2010-11/2013	Katanov Khakas State University PhD student, 20.11.2013 - Candidate of Physico-Mathematical Sciences (Equivalent to Ph.D., Condensed Matter Physics). Thesis: Molecular dynamics simulations synthesis of Cu nanoparticles from the gas phase (Supervisor: Yuri Ya. Gafner, yurigafner@gmail.com)	Abakan, Russia
9/2005 - 8/2010	Katanov Khakas State University Basic classical education, Physics	Abakan, Russia

ADVANCED SCHOOLS

2/2014-3/2014	Forschungszentrum Jülich, Peter Grünberg Institute 45 th IFF Spring School "Computing Solids: Models, Ab-initio Methods and Supercomputing"	Jülich, Germany
3/2015	Forschungszentrum Jülich, Peter Grünberg Institute 46 th IFF Spring School "Functional Soft Matter"	Jülich, Germany
3/2019	Forschungszentrum Jülich, Peter Grünberg Institute 46 th IFF Spring School "Scattering! Soft, Functional and Quantum Materials"	Jülich, Germany

AWARDS and PRIZES

2016	The third place for the report at the XIII International Conference of Students and Young Scientists "Prospects of Fundamental Sciences Development", National Research Tomsk Polytechnic University, Tomsk, Russia
2012-2013	Special state scholarship of Russian Federation Government 2012/13. The Order of Ministry of Education and Science of the Russian Federation №935 from 19.11.2012

2012	Certificate for the best report at the XVIII Russian conference of students and young scientists physicists (VNKSF-18), Siberian Federal University, Krasnoyarsk, Russia
2012	Award of the Government of the Republic of Khakassia in the category "Young researcher"
2011	The first place for the report at the VIII International Conference of Students and Young Scientists "Prospects of Fundamental Sciences Development", National Research Tomsk Polytechnic University, Tomsk, Russia
2010	The first place in the Republican competition of scientific – research works of students of higher educational institutions, Abakan, Russia
2010	Russian President Student Award for supporting talented young students.
2010	Award of the Government of the Republic of Khakassia in the category "Young researcher", Abakan, Russia
2009	The first place in the Republican competition of scientific – research works of students of higher educational institutions, Abakan, Russia

GRANT HELD

1. Russian Science Foundation (Project 22-73-00219) [2022-2024]: «Computer design of new electrolytes for solid-state batteries», **Principal Investigator**. (Russia)
2. German Academic Exchange Service- DAAD program "Mikhail Lomonosov" [2020-2021]: «*Prospective materials for the anodes of high-capacity metal-ion batteries from first-principles computer simulations*», **Principal Investigator**. (Germany)
3. German Academic Exchange Service- DAAD program "Mikhail Lomonosov" [2018-2019]: «*Atomistic simulations of impacts of high-energy ions on two-dimensional transition metal dichalcogenides within the framework of a two-temperature model*», **Principal Investigator**. (Germany)
4. Program of Foundation for promoting the development of small enterprises in scientific and technical sphere, *UMNIK* program [2017-2018]: «*Development of a software package for optimization of synthesis parameters for nanopowders of metals and alloys*», **Principal Investigator**. (Russia)
5. Prokhorov Foundation grant, «*Academic Mobility*» program [2017], **Principal Investigator**. (Russia)
6. Grant of Russian Foundation for Basic Research (Russia)
 - a. [2017-2018], #17-42-190308_r: «*Complex experimental and theoretical investigation of iron and manganesilicides epitaxial thin films*», **Principal Investigator**;
 - b. [2016-2017], #16-48-190182_r: «*Development of some technological aspects for creation stable metal nanoobjects and some technical devices on their basis*», co-P.I.;
 - c. [2016-2017], #16-32-000125-mol_a: «*Investigation of synthesis mechanisms and thermal properties of homogeneous and heterogenous bicomponent nanoparticles*», **Principal Investigator**;
 - d. [2015-2016], #15-42-04164_r_sibir'_a: «*Creation of the ordered structures from nanodispersed particles condensed from a gas phase*», co-P.I.;
 - e. [2013-2014], #13-02-98000_r_sibir'_a: «*Creation of experimental-theoretical bases for synthesis of nanopowders of metals, oxides, nitrides synthesized after condensation of high temperature vapor*», co-P.I.;
 - f. [2012-2013], #12-02-98000_r_sibir'_a: «*Development of the theory for creation stable nanostructures on the basis of metal clusters under condition of external influence various nature*», co-P.I.;
 - g. [2012], #12-02-90804-mol_rf_nr: «*The thermal stability of ensembles of nanoclusters Ir and Ru on SiO₂ substrate and grapheme*», **Principal Investigator**;
 - h. [2011-2012], #11-02-98006_r_sibir'_a: «*Creation of theoretical bases for synthesis of metal nanoparticles from the gas environment*», co-P.I.;
 - i. [2009-2010], #09-02-98000_r_sibir'_a: «*Development of the theory of metal nanoparticles synthesis from a high-temperature gas phase*», co-P.I.;
7. Grants of the President of Russian Federation [2009-2010], # MK_2207.2009.2: «*The development of physical and technological principles of formation of nanostructures of certain fcc metals for the catalysis and functional electronics*», co-P.I.; (Russia)
8. State Task of the Ministry of Education and Science of the Russian Federation [2014-2016]: «*Computer modeling of the theoretical foundations of the production of nanostructures of fcc metals, stable, subject to various external influences*» co-P.I.; (Russia)

WORKSHOPS and CONFERENCES (PROFESSIONAL and SCIENTIFIC MEETING)

- 4/2025** V Russian Congress on Catalysis "ROSKATALIZ" (St. Petersburg), Russia
- 10/2024** XXII Mendeleev Congress on General and Applied Chemistry, Sochi (Federal Territory "Sirius"), Russia

- 08/2023** 26th Congress and General Assembly of the International Union of Crystallography (IUCr 2023), Melbourne, Australia
- 6/2019** Inaugural Symposium for Computational Materials Program of Excellence (CMP Symposium), Skoltech, Moscow, Russia
- 5/2019** Workshop «Application of Machine-Learning Interatomic Potentials in Materials Design», Moscow, Russia
- 3/2019** Physics Boat Workshops (PBW - 2019), poster session «Atomic structure and electronic properties of few-atom alkali metal between two graphene and MoS₂ sheets», Helsinki, Finland - Stockholm, Sweden
- 2/2019** 50th IFF Spring School Scattering! Soft, Functional and Quantum Materials, poster session, «Atomic structure and electronic properties of few-atom Li, Na, K layers between two graphene and MoS₂ sheets», Jülich, Germany
- 8/2018** Towards Reality in Nanoscale Materials X, poster session, «Atomic structure and electronic properties of few-atom sodium and potassium layers between two graphene sheets», Levi, Finland.
- 3/2017** XXVII International Materials Research Congress, «Computer investigation of synthesis, structural and electronic properties of bimetallic nanoparticles» **Invited Speaker**, Cancun, Mexico.
- 4/2016** Seminar «Computer simulation of nanoparticles», Technological Institute for Superhard and Novel Carbon Materials, Moscow, Russia
- 6/2016** XIII International Conference of Students and Young Scientists "Prospects of Fundamental Sciences Development", National Research Tomsk Polytechnic University, Tomsk, Russia
- 2/2015** International Scientific and Technical Conference Nanotechnologies of Functional Materials (NFM'16), Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russia
- Seminar Laboratory of Physics of the magnetic phenomena «Theoretical modeling of thermal effects on the copper nanoparticles», L.V. Kirensky Institute of Physics, Krasnoyarsk, Russia
- 9/2014** IV Interdisciplinary International Symposium «The physics of surface phenomena, phase boundaries and phase transitions» (PSP&PT), Tuapse, Russia
- 11/2012** All-Russian Youth Conference «Physics and chemistry of nanoscale systems», Ural Federal University, Ekaterinburg, Russia
- 3/2012** XVIII Russian conference of students and young scientists physicists (VNKSF-18), Siberian Federal University, Krasnoyarsk, Russia
- 9/2011** XIII International Conference «Opto, nanoelectronics, nanotechnologies and microsystems», Ulyanovsk State University, Abrau-Durso, Russia
- 6/2011** 9th International Scientific Conference «Advanced metal materials and technologies» (AMMT'2011), Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russia
- 4/2011** VIII International Conference of Students and Young Scientists «Prospects of Fundamental Sciences Development», National Research Tomsk Polytechnic University, Tomsk, Russia
- 11/2010** XI All-Russian School-Seminar on Physics of Condensed Matter (SPFKS-11), Institute of Metal Physics, Ekaterinburg, Russia
- 9/2010** XI International Workshop «Evolution of the defect structure in Condensed Matter», Altai State Technical University, Barnaul, Russia
- 4/2010** XLVIII International Scientific Student Conference «Student and technological progress», Novosibirsk State University, Novosibirsk, Russia
- 2/2010** 2th All-Russian seminar «Physics and chemistry of surfaces and nanostructures», A.N. Frumkin Institute of Physical chemistry and Electrochemistry RAS, Moscow, Russia
- 10/2009** X All-Russian School-Seminar on Physics of Condensed Matter (SPFKS-10), Institute of Metal Physics, Ekaterinburg, Russia
- 5/2009** VI International Conference of Students and Young Scientists «Prospects of Fundamental Sciences Development», National Research Tomsk Polytechnic University, Tomsk, Russia

REFeree FOR SCIENTIFIC JOURNALS

Journal of Alloys and Compounds, Industrial & Engineering Chemistry Research, Journal of Molecular Liquids, Computational Materials Science

PUBLICATIONS

1. **Chepkasov I.V.**, Kvashnin A.G. Multilayers Alkali Metal Structures a Way to High Capacity and Fast Charging Carbon-Based Metal-Ion Battery. A Review // Small. 2025. e08433. **(D1)**
2. **Chepkasov I. V.**, Baidyshev V. S., Kvashnin A. G. Core-dictated tuning of the performance of amorphous and crystalline TM@Pt and HEA@Pt core-shell nanoparticles catalysts // Materials Today Energy. 2025. 54. 102130. **(D1)**

3. Dallakyan O. L., Maltsev A. P., **Chepkasov I. V.**, Aghamalyan M. A., Hunanyan A. A., Petrosyan N. Z., Chobanyan M. S., Sahakyan M. T., Khachatryan L. G., Oganov A. R., Zakaryan H. A. Computational screening for novel solid-state electrolytes in Li₃MX₃ composition // *Journal of Energy Chemistry*. 2026. 112. 495-504. (D1)
4. Bayan Y. A., Beskopylny E. R., Gerasimov E. U., Aydakov E. E., Volik K. K., Pankov I. V., **Chepkasov I. V.**, Lukanov M. M., Kvashnin A. G., Alekseenko A. A. Boosting the Performance of Pt/C Catalysts via Nitrogen-Doped Carbon Support: Insights from Structural and Electrochemical Characterization // *Small*. 2025. e10144. (D1)
5. Vildanova A. R., Goldt A. E., Porokhin S. V., Kvashnin A. G., Baidyshev V. S., **Chepkasov I. V.**, Fedorov F. S., Litvintseva K. A., Lalov A. V., Dmitrieva V. A., Teplakova M. M., Nasibulin A. G. Encapsulated Nickel Nanowires Inside Plasma-treated Single-Walled Carbon Nanotubes for Urea Oxidation // *Small*. 2025. 21. e07040. (D1)
6. **Chepkasov I. V.**, Radina A. D., Baidyshev V. S., Polovinkin M., Rybin N., Shapeev A., Krikorov A. A., Oganov A. R., Dashevsky Z., Kvashnin D. G., Kvashnin A. G. Tuning of mechanical properties of doped PbTe-based thermoelectric materials driven by intrinsic defects // *Journal of Materials Chemistry A*. 2025. 13. 31170-31181. (D1)
7. **Chepkasov I. V.**, Baidyshev V. S., Iosimovska A. V., Zamulin I. S., Kvashnin A. G. Adsorption properties of crystalline and amorphous PdIr nanoparticles. A systematic first-principles study // *Journal of Catalysis*. 2025. 447. 116102. (Q1)
8. Maltsev A. P., Iosimovska A. V., **Chepkasov I. V.**, Oganov A. R. Structure transformations and ionic conductivity in germanides of sodium and potassium // *Journal of Materials Chemistry A*. 2025. 13. 14612-14619. (D1)
9. **Chepkasov I. V.**, Baidyshev V. S., Kvashnin A. G. Polyaromatic hydrocarbons as prospective anode materials for metal ion battery // *Journal of Energy Storage*. 2025. 125. 116831. (D1)
10. Burganova R. M., Umar Z., Nedopekin O. V., **Chepkasov I. V.**, Piyanzina, I. I. Complex investigation of XF₃ (X= Gd, Tb, Dy, Ho and Er) fluorides under pressure: An ab-initio perspective // *Computational Materials Science*. 2025. 246. 113428. (Q1)
11. Radina A. D., Baidyshev V. S., **Chepkasov I. V.**, Matsokin N. A., Altalhi T., Yakobson B. I., Kvashnin A. G. Theoretical study of adsorption properties and CO oxidation reaction on surfaces of higher tungsten boride // *Scientific Reports*. 2024, 14, 1, 12788. (Q1)
12. Iosimovska A. V., Maltsev A. P., **Chepkasov I. V.**, Oganov A. R. Thermodynamic Stability and Ionic Conductivity in Lithium-Germanium Binary System // *Applied Physics Letters*. 2024, 124, 16. (Q1)
13. **Chepkasov I. V.**, Radina A. D., Kvashnin A. G. Structure-driven tuning of catalytic properties of core-shell nanostructures // *Nanoscale*. – 2024, 16, 5870-5892 (Q1)
14. **Chepkasov I. V.**, Kvashnin A. G., Radina A. D., Matsokin N. A., Jalolov F. N., Kvashnin D. G., Oganov A. R. Dashevsky Z. Origin of brittle behavior of doped PbTe-based thermoelectric materials // *Applied Physics Letters*. 2024, 124, 2. (Q1)
15. Maltsev A. P., **Chepkasov I. V.**, Oganov A. R. New promising class of anode materials for Ca-ion battery: polyaromatic hydrocarbons // *Materials Today Energy*. 2024, 39, 101467. (D1)
16. **Chepkasov I. V.**, Zamulin I. S., Baidyshev V. S., Kvashnin A. G. Tuning the surface properties of AuPd nanoparticles for adsorption of O and CO // *Physical Chemistry Chemical Physics*. 2023, 25, 48, 33031-33037. (Q1)
17. **Chepkasov I. V.**, Baidyshev V. S., Kvashnin A. G. Structure-driven tuning of O and CO adsorption on AuCu nanoparticles: A density functional theory study // *Physical Review B*. 2023, 108, 20, 205414. (Q1)
18. Maltsev A. P., **Chepkasov I. V.**, Oganov A. R. Order–Disorder Phase Transition and Ionic Conductivity in a Li₂B₁₂H₁₂ Solid Electrolyte // *ACS Applied Materials & Interfaces*. 2023, 15, 36, 42511-42519. (D1)
19. **Chepkasov I. V.**, Krasheninnikov A. V. Tetracene crystals as promising anode material for alkali metal ion batteries // *Carbon*. 2023, 118190. (D1)
20. Maltsev A. P., **Chepkasov I. V.**, Kvashnin A. G., Oganov A. R. Ionic Conductivity of Lithium Phosphides // *Crystals*. 2023, 13, 5, 756.
21. Zhou D., Semenok D. V., Volkov M. A., Troyan I. A., Seregin A. Yu., **Chepkasov I. V.**, Sannikov D. A., Lagoudakis P. G., Oganov A. R., German K. E. Synthesis of technetium hydride TcH_{1.3} at 27 GPa // *Physical Review B*. 2023, 107, 6, 064102. (Q1)
22. Leybo D., Firestein K. L., Evdokimenko N. D., Ryzhova A. A., Baidyshev V. S., **Chepkasov I. V.**, Popov Z. I., Kustov A. L., Konopatsky A. S., Golberg D. V., Shtansky D. V. Effect of ball-mill processing on catalytic activity and selectivity of Fe/h-BN catalysts for CO₂ hydrogenation // *ACS Applied Nano Materials*. 2022, 5, 11, 16475-16488. (Q1)
23. **Chepkasov I. V.**, Baidyshev V. S., Golubnichiy A. A., Zamulin I. S., Kvashnin A. G., Kozlov S. M. Cu–Au nanoparticles produced by the aggregation of gas-phase metal atoms for CO oxidation // *Aggregate*. 2022, e273. (D1)
24. **Chepkasov I. V.**, Smet J. H., Krasheninnikov A. V. Single- and Multilayers of Alkali Metal Atoms inside Graphene/MoS₂ Heterostructures: A Systematic First-Principles Study // *The Journal of Physical Chemistry C*. 2022, 126, 37, 15558–15564 (Q1)
25. Rybin N., **Chepkasov I. V.**, Novoselov D. Y., Anisimov V. I., Oganov A. R. Prediction of Stable Silver Fluorides // *The Journal of Physical Chemistry C*. 2022, 126, 35, 15057–15063. (Q1)

26. Kvashnin A. G., Nikitin D. S., Shanenkov I. I., **Chepkasov I. V.**, Kvashnina Y. A., Nassyrbayev, A., Sivkov A. A., Bolatova Z., Pak A. Ya. Large-Scale Synthesis and Applications of Hafnium–Tantalum Carbides // *Advanced Functional Materials*. 2022. 2206289. (D1)
27. Wang, Y., Bykov, M., **Chepkasov, I.V.**, Samtsevich, A., Bykova, E., Zhang, X., Jiang S., Greenberg E., Chariton S., Prakapenka V. B., Oganov A. R., Goncharov, A. F. Stabilization of hexazine rings in potassium polynitride at high pressure // *Nature Chemistry*. 2022. 14. 794–800 (D1)
28. Kovalskii A. M., Volkov I. N., Evdokimenko N. D., Tkachenko O. P., Leybo D. V., **Chepkasov I. V.**, Popov Z. I., Matveev A. T., Manakhov A., Permyakova E. S., Konopatsky A. S., Kustov A. L., Golberg D.V., Shtansky D. V. Hexagonal BN-and BNO-supported Au and Pt nanocatalysts in carbon monoxide oxidation and carbon dioxide hydrogenation reactions // *Applied Catalysis B: Environmental*. 2022. 303. 120891. (D1)
29. **Chepkasov I. V.**, Sukhanova E. V., Kvashnin A. G., Zakaryan H. A., Aghamalyan M. A., Mamasakhlisov Y. S., Manakhov A.M., Popov Z.I., Kvashnin D. G. Computational Design of Gas Sensors Based on V₃S₄ Monolayer // *Nanomaterials*. 2022. 12. 5. 774. (Q1)
30. K. L. Firestein, N. D. Evdokimenko, A. L. Kustov, V. S. Baidyshev, **I. V. Chepkasov**, Z. I. Popov, A. T. Matveev, I. V. Shetinin, D. V. Leybo, I. N. Volkov, A. M. Kovalsky, D. Golberg, D. V. Shtansky Microstructure and catalytic properties of Fe₃O₄/BN, Fe₃O₄ (Pt)/BN, and FePt/BN heterogeneous nanomaterials in CO₂ hydrogenation reaction: Experimental and theoretical insights // *Journal of Catalysis*. 2021. 402. 130-142. (Q1)
31. **Chepkasov I. V.**, Erohin S. V., Sorokin P. B. The Features of Phase Stability of GaN and AlN Films at Nanolevel // *Nanomaterials*. – 2021. 11. 1. 8. (Q1)
32. **Chepkasov I. V.**, Ghorbani-Asl M., Popov Z. I., Smet J. H., Krashenninnikov A. V. Alkali metals inside bi-layer graphene and MoS₂: insights from first-principles calculations // *Nano Energy*. 2020. 104927. (D1)
33. **Chepkasov I.V.**, Baidyshev V.S., Sukhanova E.V., Visotin M.A., Süle P., Popov Z.I. Iron silicides formation on Si (100) and (111) surfaces through theoretical modeling of sputtering and annealing // *Applied Surface Science*. 2020. 146736. (Q1)
34. Konopatsky, A.S., Leybo, D.V., Firestein, K.L., **Chepkasov, I.V.**, Popov, Z.I., Permyakova, E.S., Volkov, I.N., Kovalskii, A.M., Matveev, A.T., Shtansky, D.V., Golberg, D.V. Polyol synthesis of Ag/BN nanohybrids and their catalytic stability in CO oxidation reaction // *ChemCatChem*. 2020. 12. 6. 1691-1698. (Q1)
35. Ponomarev V., Sheveyko A. N., Permyakova E. S., Lee J., Voevodin A. A., Berman D, Manakhov A., Michlicek M., Slukin P., Firstova V., Ignatov S., **Chepkasov I. V.**, Popov Z. I., Shtansky D.V. TiCaPCON-Supported Pt-and Fe-based Nanoparticles and Related Antibacterial Activity // *ACS Applied Materials & Interfaces* 2019. 11. 32. 28699-28719 (D1)
36. **Chepkasov I. V.**, Visotin M. A., Kovaleva E. A., Manakhov A. M., Baidyshev V. S., Popov Z. I. Stability and Electronic Properties of PtPd Nanoparticles via MD and DFT Calculations // *The Journal of Physical Chemistry C*. 2018. 122. 31. 18070-18076.
37. Baidyshev V. S., **Chepkasov I. V.**, Artemova N. D. Study of thermal stability of disordered alloy Ag_xCu_{1-x} nanoparticles by molecular dynamic simulations // *Journal of Physics: Conference Series*. 2018. 1015. 3. 032021.
38. **Chepkasov I. V.**, Baidyshev V. S., Baev A. Y. Structural properties of CuAu nanoparticles with different type. Molecular dynamic simulations // *Journal of Physics: Conference Series*. 2018. 1015. 3. 032022.
39. **Chepkasov I. V.**, Baidyshev V. S., Tsura V. A. Molecular dynamic simulation of melting copper-silicon nanoparticles // *Journal of Physics: Conference Series*. 2018. 1015. 3. 032023.
40. **Chepkasov I. V.**, Gafner Yu.Ya., Visotin M.A., Redel L.V. Melting of PdPt nanoparticles of different types // *Physics of the Solid State*. 2017. 59. 10. 2076-2081.
41. **Chepkasov I. V.**, Gafner Y. Y., Gafner S. L. Synthesis of Cu nanoparticles by condensation from the gas phase // *Phase Transitions*. 2017. 90. 6. 590-597.
42. Kurbanova E. D., Polukhin V. A., **Chepkasov I. V.** Thermostability of interface structure metal on graphene and silicene // *Letters on materials*. 2016. 6. 2. 109-112.
43. **Chepkasov I. V.**, Gafner Y. Y., Gafner S. L., Bardakhanov S. P. Condensation of Cu nanoparticles from the gas phase // *The Physics of Metals and Metallography*. 2016. 117. 10. 1003-1012.
44. **Chepkasov I. V.**, Gafner Y. Y., Gafner S. L. Changing of the shape and structure of Cu nanoclusters generated from a gas phase: MD simulations // *Journal of Aerosol Science*. 2016. 91. 33-42.
45. **Chepkasov I. V.**, Gafner Y. Y., Gafner S. L., Bardakhanov S. P. The general mechanisms of Cu cluster formation in the processes of condensation from the gas phase // *Bulletin of Materials Science*. 2015. 38. 3. 701-706.
46. **Chepkasov I. V.**, Popov Z. I. Analysis of thermal effects on copper nanoparticles synthesized from the gas phase // *IOP Conference Series: Materials Science and Engineering*. – IOP Publishing, 2015. 81. 1. 012033.
47. **Chepkasov I. V.**, Redel L. V. Calculations of the heat capacity of Cu clusters synthesized by condensation from the gas phase // *IOP Conference Series: Materials Science and Engineering*. – IOP Publishing. 2015. 81. 1. 012014.
48. **Chepkasov I. V.**, Gafner Yu.Ya., Gafner S.L. Role of the Clusters' Boundaries in the Calculations of the Heat Capacity of Cu Clusters Synthesized from the Gas Environment // *Quantum Matter*. 2014. 3. 1. 78-83.

49. **Chepkasov I. V.**, Gafner Yu.Ya., Kurbanova E.D., Polukhin V.A. Study of the effect of ultrafast heating on the structure and shape of the gas phase synthesized Cu nanoparticless // Letters on materials. 2014. 4. 4. 249-252.
50. Polukhin V. A., Gafner Y. Y., **Chepkasov I. V.**, Kurbanova E. D. Comparative analysis of the thermosize effects of transition-metal clusters that are free or deposited onto graphene. Molecular dynamics simulation //Russian Metallurgy (Metally). 2014. 2014. 2. 112-125.
51. **Chepkasov I.V.**, Gafner Yu.Ya., Gafner S.L. Analysis of the impact of thermal effects on the structural evolution of nanoclusters Cu and Ni // Russian Physics Journal. 2011. 54. 1/3. 318 - 324.
52. Gafner Y. Y., Gafner S. L., **Chepkasov I. V.** The effect of thermal treatment on the organization of copper and nickel nanoclusters synthesized from the gas phase //Journal of Experimental and Theoretical Physics. 2010. 111. 4. 608-618.