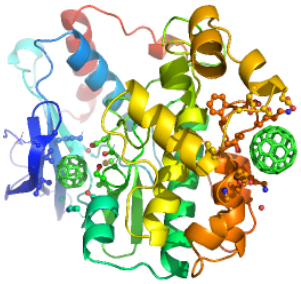

International Conference on
Computational Science and Technology
ICCST 2014

May 15-16, 2014
Warsaw, Poland

Book of Abstracts

Institute of Physics Polish Academy of Sciences

Al. Lotników 32/46 Warsaw, Poland

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Computational Chemistry

Material Science

Protein Folding and Misfolding

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A.M. Gabovich, Institute of Physics NASU, Kiev, Ukraine

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Vinh Hung Tran, ILTSR PAS, Wroclaw , Poland

Thuat T. Trinh, NUST, Trondheim, Norway

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Conference venue

Conference room, Institute of Physics Polish Academy of Sciences,

Al. Lotnikow 32/46, Warsaw, Poland

Programme

Thursday, 15 May 2014

8:30-9:40 Registration

9:40-10:00 Opening Section

SECTION I Computational Chemistry and Material Science

Chairperson: Duc Nguyen-Manh

10:00-10:30 Minh Tho Nguyen, University of Leuven, Belgium

Computational Quantum Chemistry at Leuven

10:30-11:00 Truong Ba Tai, University of Leuven, Belgium

Disk-aromaticity and its application for polycyclic compounds

11:00-11:30 *Coffee Break*

Chairperson: Minh Tho Nguyen

11:30-12:00 S. Roszak, Wrocław University of Technology, Poland

Quantum chemistry – the efficient first step for designing materials of desired properties

12:00-12:30 Thuat T Trinh, Norwegian University of Science and Technology, Trondheim, Norway

Prediction of Chemical Potential and Activity Coefficient of Graphite Surface from Molecular Dynamics Simulation

12:30-13:00 Duc Nguyen-Manh, Culham Centre for Fusion Energy, UK

Integrated modeling approach for nuclear fusion, material science and engineering

13:00-14:30 **Lunch and Poster Section**

Chairperson: S. Roszak

14:30-15:00 Vu Thi Ngan, Qui Nhon University, Vietnam

Interesting properties found in doped silicon clusters

15:00-15:30 R. Buczko, Institute of Physics PAS, Warsaw, Poland

Surface states of topological crystalline insulators

15:30-16:00 *Coffee Break*

16:00-16:30 Alesander Gabovich, Institute of Physics NASU, Kiev, Ukraine

Stationary Josephson current between d-wave superconductors with charge density waves: angular dependences and violations of the corresponding-states relationship

16:30-17:00 Vinh Hung Tran, Institute of Low Temperature and Structure Research PAS, Wroclaw, Poland

Electronic Structure of Selected Strongly Correlated Electron Systems

19:00-22:00 CONFERENCE BANQUET

Friday 16 May 2014

SECTION II COPUTATIONAL BIOPHYSICS AND MEDICINE

Chairperson: Mai Suan Li

9:30-10:00 Andrzej Koliński, University of Warsaw, Poland

CABS - coarse grained modeling of protein structure assembly, dynamics and interactions

10:00-10:30 Bartosz Rozycki, Institute of Physics PAS, Warsaw, Poland

Ensembles of multi-protein complexes in simulation and experiment

10:30-11:00 Maksim Kouza, University of Warsaw, Poland

Molecular Dynamics Simulations of Forced Protein Unfolding

11:00-11:30 *Coffee Break*

Chairperson A. Kolinski

11:30-12:00 Slawomir Filipek, University of Warsaw, Poland

Activation Routes of G-Protein-Coupled Receptors

12:00-12:30 Phuong Hoang Nguyen, Institute of Biophysical Chemistry, CNRS, Paris

Structures and dynamics of Aβ oligomers and their interactions with known inhibitors

12:30-13:00 Tap Ha-Duong, University Paris-Sud, Châtenay-Malabry, France

Coarse-grained molecular modeling of the membrane receptor CXCR4 recognition by the chemokine CXCL12

13:00-14:30 **Lunch and Poster Section**

Chairperson: Phuong Hoang Nguyen

14:30-15:00 Sebastian Kmiecik, University of Warsaw, Poland

Introduction to CABS-based tools for protein modeling: CABS-flex, CABS-fold and py-CABS

15:00-15:30 Trung Hai Nguyen, Forschungszentrum Jülich GmbH, Germany

Cisplatin binding to proteins: insights from molecular simulation

15:30-16:00 Mai Suan Li, Institute of Physics PAS, Warsaw, Poland

Protein aggregation: Insights from lattice models

Saturday, 17 May 2014

From 9:30 Excursion

Remark: All posters will be viewed during the whole time of the conference. Please, place your poster immediately after arrival and dismount it not earlier than after the closing lecture.

INVITED TALKS

SECTION I Computational Chemistry and Material Science

I1. Computational Quantum Chemistry at Leuven

Minh Tho Nguyen

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We will present an overview of the theoretical/computational work which is being carried out in our research group at KU Leuven. This includes the projects in different fields:

- Chemical concepts (such as the aromaticity)
- High accuracy computations on thermochemical parameters of small molecules,
- Prebiotic, atmospheric and combustion chemistries,
- Theoretical design of conjugated polymers,
- Structural and spectroscopic signatures of the elemental clusters,
- Building of force fields for probing reactions in solid state.

I2. Disk-aromaticity and its application for polycyclic compounds

Truong Ba Tai

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Aromaticity is one of the most widely discussed concepts in chemistry. Initially introduced to interpret the high stability of planar and -conjugated monocyclic hydrocarbons [1], aromaticity has nowadays extensively been applied for other types of compounds such as heterocyclic compounds [2], polycyclic organic compounds [3], inorganic complexes, atomic clusters of elements [4;5]. In this presentation, we showed that the aromaticity of polycyclic compounds can be rationalized by using a simple model of a particle in a circular box. The model of a particle on a ring provides a simple conceptual approach to the electronic structure of annular molecules. The two-dimensional analogue of the ring model is a circular disk model. It is expected to be applicable to planar molecular arrays with a circular shape.

References:

[1] Kekule A (1865) Bull Soc Chim Paris 3: 98 110

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[3] Watson MD, Fechtenktter A, Mullen (2001) Chem Rev 101: 1267 1300.

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I3. Quantum chemistry - the efficient first step for designing materials of designed materials

Szczepan Roszak

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The application of quantum-chemical methodology is illustrated for modelling materials with predefined physical and chemical properties. Carbon based materials for the hydrogen storage, conducting polymers, and dye-sensitized solar cells are studied with the arm to relate fundamental insight with experiment and technology useful data.

I4. Prediction of Chemical Potential and Activity Coefficient of Graphite Surface from Molecular Dynamics Simulation

Thuat T.Trinh, [a] Dick Bedeaux, [a] and Signe Kjelstrup [a,b]
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b) Department of Process and Energy, Delft University of Technology, Delft, Netherlands
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Method to calculate thermodynamic properties of macroscopic systems by extrapolating properties of systems of molecular dimensions was recently developed in Signe and Dicks group.[1;2] Appropriate scaling laws for small systems were derived using the method for small systems thermodynamics of Hill, considering surface and nook energies in small systems of varying sizes. The method can be us ed to compute thermodynamic data for the macroscopic limit from knowledge of fluctuations in various bulk systems. [3;4]

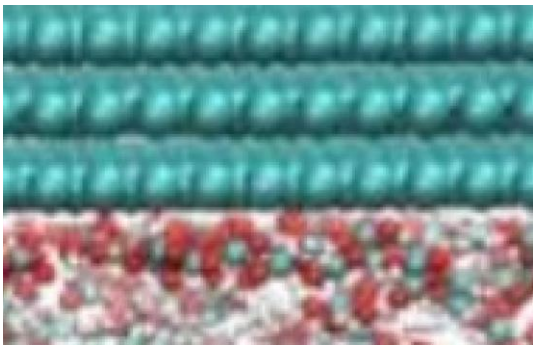

Figure 1 Typical snapshot of the gas mixture of CO_2 and H_2 in equilibrium with the carbon membrane with poresize W gas mixture CO_2: H_2 (mole fraction $^{x}CO_2$ = 0:3). The green, red and white are represented carbon, oxygen and hydrogen atom, respectively.

Here we can apply this small system method for a graphite surface system with CO2 adsorbed [5] or CO_2 - H_2 mixture adsorbed (Figure 1). From Equilibrium Molecular Dynamics simulation data , we predicted the chemical potential and activity coefficient of the surface in various temperature and pressure conditions.

References:

[1] Schnell, S. K.; Liu, X.; Simon, J.-M.; Bardow, A.; Bedeaux, D.; Vlugt, T. J. H.;Kjelstrup, S. Journal of Physical Chemistry B (2011), 115, 10911.

[2] Schnell, S. K.; Vlugt, T. J. H.; Simon, J.-M.; Bedeaux, D.; Kjelstrup, S. Mol. Phys. 2011, 110, 1069.

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I5. Integrated Modeling Approach for Nuclear Fusion Materials Science and Engineering

Duc Nguyen-Manh

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The performance demands on different components of future tokamak-based fusion power plants are beyond the capacity of current materials which is one of the reasons that the United States National Academy of Engineering has ranked the quest for fusion as one of the top grand challenges for engineering in the 21st century. These challenges are even more outstanding by the lack of experimental testing facilities that replicate the extreme operating environment involving simultaneous high heat and particle uxes, large time-varying stresses, corrosive chemical environments, and large fluxes of 14-MeV peaked fusion neutrons. Fortunately, recent innovations in theoretical and modeling methodologies, increasingly powerful high-performance and massively parallel computing platforms,

and improved analytical experimental characterization techniques provide the means to develop self-consistent, experimentally validated designs of materials performance and degradation in the fusion energy environment. This talk will describe new integrated approach combining reliable results based on density-functional theory modelling of radiation damage with neutron transmutation and inventory calculations for predicting the critical component lifetimes associated with the helium-induced grain-boundary embrittlement of materials.

This work, part-funded by the European Communities under the contract of Association between EURATOM and CCFE, was carried out within the framework of the European Fusion Development Agreement. To obtain further information on the data and models underlying this paper please contact Publication-Manager@ccfe.ac.uk. The views and opinions expressed herein do not necessarily reflect those of the European Commission. This work was also part-funded by the RCUK Energy Programme under grant EP/I501045.

DNM would like to the International Fusion Energy Research Centre (IFERC) for using the supercomputer (Helios) at Computational Simulation Centre (CSC) in Rokkasho (Japan).

I6. Interesting properties found in doped silicon clusters

Vu Thi Ngan,[1] Minh Tho Nguyen[2]

[1] *Faculty of Chemistry, Quy Nhon University,170 An Duong Vuong, Quy Nhon, Binh Dinh, Vietnam*

[2] *Department of Chemistry, University of Leuven, Belgium*

Silicon is one of the most applied elements in the semiconductor industries. With the ongoing miniaturization trend of microelectronic components, the electronic devices will soon reach down to the size of atomic clusters. However, bare silicon clusters cannot be directly used in applications since they are chemically reactive due to their dangling bonds. It is conjectured that properly doping silicon clusters with metal atoms could overcome this deficiency. In this presentation, we would like to talk about some interesting points found in Si clusters thanking to doping phenomenon. For example basket-like Si clusters possess large magnetic moment when doped with Mn or Cr; cubic structures can be formed by doping with Be, B and C; fullerene-like structures are stabilized in some cases; planar tetracoordinate C is stabilized in CSi_9 by enjoying stabilization from both electronic effect and geometrical constraint of the Si_9 cages.

I7. Surface states of topological crystalline insulators

Ryszard Buczko

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In the recent years the study of topological phenomena became one of the major topics in condensed matter physics. This was accelerated by the theoretical prediction and the successive experimental discovery of topological insulators in which the time-reversal symmetry and the inverted band structure result in the occurrence of topologically protected metallic Dirac-like electronic surface states. New theoretical developments led to a discovery of the new class of materials with similar properties, i.e., topological crystalline insulators (TCIs). In the rock-salt IV-VI crystals topological protection of metallic surface states is secured by the crystalline mirror plain symmetry [1-4]. We study the nature of surface states in the two solid solutions: $Pb_{1-x}Sn_xSe$ and $Pb_{1-x}Sn_xTe$. It has been shown that these narrow-gap semiconductors belong to TCIs for big enough Sn content and that the transition from trivial to topologically nontrivial class can be tuned by temperature [2]. Using tight binding approach for the band structure calculation, we show that the energy spectrum and the expected spin texture of the surface states strongly depends on the surface orientation [6]. Angle-resolved and spin-resolved photoelectron spectroscopy experiments, supported by the band structure calculations have proven the existence of topologically protected, spin polarized surface states with the Dirac-like dispersion on the (100) [2;5] as well as on the (111) surfaces [6] of the considered crystals.

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I8. Stationary Josephson current between d-wave superconductors with charge density waves: angular dependences and violations of the corresponding-states relationship

Alexander M. Gabovich, [1] Mai Suan Li, [2] Henryk Szymczak, [2] and Alexander I. Voitenko [1]

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Stationary Josephson tunnel current Ic was calculated for junctions made of superconductors partially gapped by biaxial or unidirectional charge density waves (CDWs) and possessing a superconducting order parameter of d-wave symmetry. Specific calculations were carried out for symmetric junctions between two identical CDW superconducting electrodes and nonsymmetric ones composed of a CDW superconductor and a conventional isotropic s-wave superconductor. The directionality of tunneling was made allowance for. In all studied cases, the dependences of I_C on the angle between the chosen crystal direction and the normal to the junction plane were found to be significantly influenced by CDWs. It was shown, in particular, that the d-wave driven periodicity of $I_C(\gamma)$ in the CDW-free case is transformed into double-period beatings depending on the parameters of the system. The results of calculation testify that the orientation-dependent patterns $I_C(\gamma)$ measured for CDW superconductors allow the CDW configuration (unidirectional or checkerboard) and the symmetry of superconducting order parameter to be determined.

It was shown that when CDWs are absent or weak, there exists an approximate proportionality between $I_C(x)$ and the product of superconducting energy gaps $\Delta(x)$ and $\Delta(x0)$ to the left and to the right of the tunnel barrier. Here, x is either the reduced temperature, $T=T_C$, where T_C is the critical temperature of the superconducting transition, or one of the parameters characterizing the combined CDW superconducting phase. However, provided a high directionality of tunneling, CDWs may violate the law of corresponding states. The proposed method is an additional one to detect CDWs in cuprates along with the measurements of $I_C(\gamma)$ dependences.

I9. Electronic Structure of Selected Strongly Correlated Electron Systems

Vinh Hung Tran

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In strongly correlated electron (SCE) systems, where the electron-electron interactions are crucial, new physical phenomena including heavy-fermion, quantum critical points, non-Fermi liquid behaviour, unconventional superconductivity, and so on, are often observed. In order to bring insight into new problems in these materials, in addition to technologically sophisticated experiments, the band structure calculations are highly desired. The advantage of the theoretical studies is that not only may help in understanding how the matter behaves, but may predict some physical properties without reference to expensive experiments. For the considered systems, the most successful methods of the electronic structure calculations are those based on Density Functional Theory. In this talk, we give a brief overview on the electronic band structures (EBS) of selected SCE compounds, which have recently investigated by the author and co-workers, namely, superconducting Mo_3Sb_7 [1;2] and $ThPt_4Ge_{12}$ [3] ferromagnetic $U_2ScB_6C_3$ [4] and URhGe [5], and ferrimagnetic Kondo lattices Ce_5CuPb_3 [6] and Ce_5CuBi_3 [7]. The EBS have been obtained with the full-potential linearized-augmented-plane-wave and full-potential local-orbital methods, using the WIEN2k [8] and FPLO [9] packages, respectively.

References:

[1] V.H. Tran et al. Phys. Rev. Lett. 100, 137004 (2008).

[2] V.H. Tran et al. Acta Mater. 56, 5694 (2008).

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SECTION II COPUTATIONAL BIOPHYSICS AND MEDICINE

I10. CABS - coarse grained modeling of protein structure assembly, dynamics and interactions

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It is widely recognized that atomistic Molecular Dynamics (MD), a classical simulation method, captures the essential physics of protein dynamics. That idea is supported by a theoretical study showing that various MD force fields provide a consensus picture of protein fluctuations in aqueous solution. However, atomistic MD cannot be applied to most biologically relevant processes due to its limitation to relatively short time scales. Much longer time scales can be accessed by properly designed coarse-grained models. We demonstrate [1] that the aforementioned consensus view of protein dynamics from short (nanosecond) time scale MD simulations is fairly consistent with the dynamics of the coarse-grained protein model - the CABS model. The CABS model employs stochastic dynamics (a Monte Carlo method) and a knowledge-based force-field, which is not biased toward the native structure of a simulated protein. Since CABS-based dynamics allows for the simulation of entire folding (or multiple folding events) in a single run, integration of the CABS approach with all-atom MD promises a convenient (and computationally feasible) means for the long-time multiscale molecular modeling of protein systems with atomistic resolution. Combination of coarse grained simulations with MD allows also for modeling of entire protein folding processes [2].

References:

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[2] S. Kmiecik, D. Gront, M. Kouza & A. Kolinski, J. Phys. Chem. B 116:7026-7032 (2012).

[3] S. Kmiecik & A. Kolinski, J. American Chem. Soc. 133:10283-10289 (2011).

I11. Ensembles of multi-protein complexes in simulation and experiment

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Many biological functions are carried out by large and dynamic multi-protein complexes. These complexes often from only transiently and are held together by relatively weak pairwise interactions and by intrinsically disordered linkers. It is usually very difficult to derive atomic models for such protein complexes: They are not directly accessible to X-ray crystallography due to the presence of highly disordered and dynamic segments (although their separate domains can be crystallized); they are also not accessible to protein NMR due to their large molecular weights, usually above 100 kDa, which is beyond the possibilities of contemporary NMR techniques; and their inherent exibility and the lack of symmetries make them practically inaccessible to cryoEM. In the attempt to overcome these difficulties, we have developed an ensemble refinement method that combines coarse-grained molecular simulations with X-ray crystallography, small angle X-ray scattering (SAXS), spin-label distance measurements (EPR), and single-molecule fluorescence resonance energy transfer (FRET) experiments. We have applied the method to obtain detailed representations of the structures and motions in systems ranging from the ESCRT membrane-protein trafficking system to multi-domain kinases and kinases in dynamic complexes with phosphatases.

I12. Molecular Dynamics Simulations of Forced Protein Unfolding

Maksim Kouza

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One of the functional features of proteins is a response to a wide range of applied forces. In this talk I will present the results of mechanical unfolding studies for two key proteins subjected to mechanical stress, Titin and DDFLN4. We used molecular dynamic simulations at different level of resolution to investigate the mechanism of unfolding over a wide range of pulling velocities. For the first time it is reported the atomistic protein unfolding all-atom simulations in explicit solvent at near-experimental conditions. The mechanical unfolding pathways will be provided and compared. The limitation and advantages of different models will be discussed and possible extension outlined.

I13. Activation Routes of G-Protein-Coupled Receptors

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G protein coupled receptors (GPCRs), also called 7TM receptors from seven transmembrane domains, form a huge superfamily of membrane proteins that, upon activation by extracellular signals, physical or chemical, pass the signal to the cell interior. More than 800 human GPCRs allow cells to recognize diverse extracellular stimuli (photons, odorants, hormones, lipids, neurotransmitters, etc.) and transduce the signals across the plasma membrane to regulate essential physiological processes. Upon activation they pass the signal to the mediating proteins which is G protein but also arrestin. Family of GPCRs is a major class of membrane signaling proteins so these receptors are pharmacological targets for over 30% of currently used drugs.

At present, the structures of about 20 different types of GPCRs are known due to progress in micro-crystallography and in mutational thermal stabilization of these proteins. However, details of the structural and dynamical transitions within the receptors during transmembrane signaling are still unknown. The process of receptor activation consists of actions of so-called molecular switches buried in the receptor structure [1] and can lead to a wide range of activated or semi-activated structures depending on ligand bound.

We performed molecular dynamics studies of several GPCRs including N-formyl-peptide receptor (FPR1) [2], lipid receptor S1P1 [3] and μ-opioid receptor (μOR) [4]. We found that the extra-cellular pocket of FPR1 can be divided into two zones, namely, the anchor and activation regions. A mechanism was proposed concerning the initial steps of FPR1 activation concurrent with ligand binding. For FPR1 and S1P1 it was found that water molecules entering the receptor upon agonist binding are necessary for subsequent activation states. For μOR the MD simulations resolved the experimentally found dual role of sodium ions (i) to decrease the binding a_nity for agonists, and (ii) to facilitate G protein activation. Sodium ions can facilitate the activation of μOR by inducing the movement of water molecules towards the allosteric site which inuence an action of the orthosteric agonist. We also developed a GPCRM server [5] for construction of homology models of GPCRs that can be used for activity studies and also drug design purposes.

References:

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I14. Structures and dynamics of A_ oligomers and their interactions with known inhibitors

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The major component of senile plaques in the cortex and hippocampus of the brain of Alzheimer's patients is a small protein of 39-43 amino acids called amyloid beta (Aβ). A large body of experimental data points to the early Aβ formed oligomers as the primary toxic species in Alzheimer's disease, through the implication of fibril fragmentation cannot be ignored . Despite extensive experimental efforts, researcher have not been able to characterize the structures of these transient oligomers. Remarkably some mutations in Aβ either promote or prevent the disease. Some inhibitors are also known to reduce the cytotoxic effects. In this talk, I will present computer simulations can tell us about the structures and thermodynamics of small oligomers of Aβ wild type sequence and "protective" mutants in aqueous solution or interacting with potential inhibitors.

I15. Coarse-grained molecular modeling of the membrane re ceptor CXCR4 recognition by the chemokine CXCL12

Tap Ha-Duong

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CXCR4 belongs to the class A G-Protein-Coupled-Receptors family and its endogenous specific ligand is the chemokine CXCL12. It has been demonstrated that the CXCR4-CXCL12 axis plays, among other functions, a key role in the regulation of HIV infection and breast cancer metastasis [1]. Thus it has a great importance in pharmaceutical research.

The three-dimensional structure of the CXCR4 receptor has been recently solved by X-ray diffraction [2], but the _rst twenty-six amino acids of the N-terminus are missing in this structure, whereas they are one of the putative binding sites of CXCL12. In addition, NMR experiments have determined the solution structure of the chemokine CXCL12 complexed with the thirty-eight first residues of the N-terminal fragment of CXCR4 [3]. Despite this information, the interactions and recognition mechanism between the whole protein CXCR4 and its ligand CXCL12 are not completely elucidated in detail.

We report here the results of coarse-grained molecular modeling studies to gain a better insight into the CXCR4-CXCL12 interactions. First, coarse-grained protein-protein docking calculations were used to generate the most probable quaternary structures of the receptor-ligand complex. Then, coarse-grained molecular dynamics simulations were performed to assess the stability and to probe the dynamics of the CXCR4-CXCL12 conformations in a membrane environment.

References:

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I16. Introduction to CABS-based tools for protein modeling: CABS-flex, CABS-fold and py-CABS

Sebastian Kmiecik, Michal Jamroz, Maciej Blaszczyk, Andrzej Kolinski

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CABS is a coarse-grained protein model that has been well tested in a wide variety of protein simulation tasks. Based on the CABS model, we recently developed automated protocols for modeling and analysis of protein dynamics and structure: CABS-flex, CABS-fold and py-CABS.

CABS-flex [1, 2] is a web server for fast simulations of short-term dynamics of globular proteins and characterization of their fluctuations (available at http://biocomp.chem.uw.edu.pl/CABSflex/). CABS-fold [3] is a web server for de novo and consensus-based prediction of protein structure (available at http://biocomp.chem.uw.edu.pl/CABSfold/). py-CABS [4] is a software package of python modules for the simulations of long-term dynamics of globular proteins (available at http://biocomp.chem.uw.edu.pl/pycabs/).

During my presentation I will shortly introduce these tools and give examples of their capabilities, usage and limitations.

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I17. Cisplatin binding to proteins: insights from molecular simulation

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Cisplatin is one of the most widely used drugs in anticancer chemotherapy. Its antitumor activity is due to the formation of stable adducts with DNA. Unfortunately, after repeated administrations of the drug, cancer cells develop resistance mechanisms, which strongly limit cisplatin's efficacy. The decreased accumulation of cisplatin by a decreased uptake and by an increased drug efflux and sequestration is among the proposed mechanisms of resistance. Interactions of cisplatin with copper transport proteins (such as Ctr1, Atox1 and ATP7A) have been found to affect the cellular up-take, distribution and efflux of cisplatin. Therefore, understanding of the Pt coordination chemistry to these proteins may help design new Pt-based compounds able to counteract drug resistance problems. In this talk, I would like to present our computational studies to predict structural determinants of the cisplatin-protein adducts. Our computational models have been validated by spectroscopic data such as NMR, CD and EXAFS. They have provided an unprecedented insight into the structural biology of cisplatin in adducts with its cellular partners.

I18. Protein aggregation: Insights from lattice models

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Fibril formation of proteins and peptides is associated with a large group of major human diseases, including Alzheimer's disease, prion disorders, amyotrophic lateral sclerosis, type 2 diabetes etc. Therefore, understanding the key factors that govern this process is of paramount importance. The fibrillogenesis of polypeptide chains depends on their intrinsic properties as well as on external conditions. Using simple lattice we show that fibril formation times are strongly correlated with hydrophobicity, charges and population of the so called fibril-prone conformation in monomer state. The higher the population the faster is the fibril elongation and this dependence may be described by a single exponential function. Our results open a new way to understand the fibrillogenesis of bio-molecules at the monomer level. We have shown that not all of proteins have the propensity to aggregation. We will also discuss the influence of environment with focus on the recently observed dual effect of crowders on aggregation rates of polypeptide chains.

Poster Section

P1. The p-conjugated P-flowers C16(PH)8 and C16(PF)8 are potential materials for organic n-type semiconductors

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Following the theme of this special issue, two new compounds, the P-flowers C16(PH)8 and C16(PF)8, are designed by us and subsequently characterized by quantum chemical computations. Their geometries and infrared signatures are analyzed and compared to those of the well-known sulflower C16S8. Their electronic structure and aromaticity are examined using the electron localization function (ELF) and also by the total and partial densities of state (DOS). Both C16(PF)6 and C16(PH)8 molecules exhibit small energy barrier of electron injection (Fe = 0.33 eV for the gold electrode for the former, and Fe = 0.1 eV for the calcium electrode for the latter), remarkably low reorganization energy and high rate of electron hopping. Thus, both theoretically designed P-flower molecules are predicted to be excellent candidates for organic n-type.

P2. Singly and doubly lithium doped silicon clusters: Geometrical and electronic structures and ionization energies

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The geometric structures of neutral and cationic SinLim0/+ clusters with n = 2 – 11 and m = 1, 2 are investigated using combined experimental and computational methods. The adiabatic (AIEs) and vertical (VIEs) ionization energies of SinLim clusters are determined using quantum chemical methods (B3LYP/6-311+G(d), G3B3 and CCSD(T)/aug-cc-pVxZ with x = D,T), whereas experimental values are derived from threshold photoionization experiments in the 4.68-6.24 eV range. Among the investigated cluster sizes, only Si6Li2, Si7Li, Si10Li, and Si11Li have ionization thresholds below 6.24 eV and could be measured accurately. The ionization threshold and VIE obtained from the experimental photoionization efficiency curves agree well with the computed values. The growth mechanism of the lithium doped silicon clusters follows some simple rules: i) neutral singly doped SinLi clusters favor the Li atom addition on an edge or a face of the structure of the corresponding Sin− anion, while the cationic SinLi+ bind with one Si atom of the bare Sin cluster or adds on one of its edges, and ii) for doubly doped SinLi20/+ clusters, the neutrals have the shape of the Sin+1 counterparts with an additional Li atom added on an edge or a face of it, while the cations have both Li atoms added on edges or faces of the Sin− clusters.

P3. Doping effects on the singlet-triplet gap and bonding of the silicon trimer

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We revisit the singlet-triplet energy gap (ΔEST) of silicon trimer and evaluate the gaps of its derivatives doped by a cation (H+, Li+, Na+, K+) and an atom (Be, Mg, Ca) using the composite G4 method, coupled-cluster theory CCSD(T)/CBS and CASPT2 (for Si3) computations. Both 1A1 and 3A2 states of Si3 are determined to be degenerate. An intersystem crossing between both states appears to be possible at a point having an apex bond angle of around α = 68 ± 2o which is 16 ± 4 kJ/mol above the ground state. The proton and alkali metal cations tend to favour the low spin state, but do not modify significantly the ΔEST, whereas a doping of earth-alkali atoms stabilize the singlet and substantially enlarge the ΔE ST of the doped clusters. The proton affinity of silicon trimer is determined as PA(Si3) = 827 ± 4 kJ/mol. The metal cation affinities and metal atom affinities are also predicted. Electron localization function (ELF) and ring current analysis shows that the singlet trimeric ring Si3 is non-aromatic, the Li+ cation renders it anti-aromatic whereas attachment of a Be atom makes the resulting tetramer a σ-aromatic cycle.

P4. Effects of Sulfur-Deficient Defect and Water on Rearrangementsof Formamide on Pyrite (100) Surface

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Pyrite (FeS2) is the most abundant and widespread sulfide mineral in the Earth's surface and in deep-see vents. In the Iron-Sulfur World scenario,1 metal sulfides (including pyrite) under hydrothermal connditions were suggested to play an important catalytic role in the synthesis of simple building blocks of life from simple molecules. Among a variety of simple chemical systems that have been investigated as prebiotic precursor, formamide (NH2CHO) has attracted a lot of interest due to several reasons. First, formamide has four important elements (N, C, O, H) for the synthesis of biomolecules. Second, formamide is an abundant molecule in the universe and its chemistry is closely related to the chemistry of HCN, a famous prebiotic precursor.2 And last but not least, formamide can decompose to form a wide range of low-molecular-weight products which facilitates the diversity of the synthesis pathways.3 Answer to the need of theoretical investigations of catalytic effects at molecular level, we set out to perform theoretical calculations of reactions of formamide on the (100) surface of pyrite. The density-functional theory (DFT) method with a plane wave-pseudopotential basis was used to study possible adsorption complexes of formamide on the ideal and sulfur-vacancy defect surfaces. Several hydrogen transfer reactions transforming formamide into its tautomers, formimic acid (NHCHOH) and aminohydroxylmethylene (NH2COH), were investigated in details. The DFT results suggest that the unimolecular hydrogen transfer reactions of formamide have high energy barrier (44-78 kcal/mol) on both ideal and defect surface. However, the reaction barriers significantly reduce with the presence of one water molecule. Reaction barriers of less than 20 kcal/mol were found for several water-assisted tautomerizations on the ideal and defect surfaces.

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P5. Surface states of the topological crystalline insulator Pb0.4Sn0.6Te

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Lately, it has been shown by angle-resolved photoelectron spectroscopy (ARPES) studies, that IV-VI substitutional alloys, Pb(1-x)SnxTe and Pb(1-x)SnxSe with Sn content x higher than a critical value, are topological crystalline insulators (TCIs) [1,2]. Very recently, spin-resolved photoelectron spectroscopy (SRPES) allowed the observation of chiral spin textures of (001) surface states in the TCI phase of these alloys [1, 3]. Here, using a tight-binding approach, we study theoretically the nature of surface states in Pb(1-x)SnxTe. The Sn content x=0.6 assures the band inversion and, thus, the newly discovered TCI phase in the (Pb,Sn)Te material. In this rock-salt TCI, the surface states with nontrivial Dirac-like energy spectrum can form at any surface of the crystal. The number of Dirac points in the surface Brillouin zone corresponds to four L-points. At least two of these Dirac points are topologically protected only at crystal surfaces symmetric about any of {110} mirror planes. These are {n n m} surfaces. We study thus, apart from the (001)-oriented surface, the surface states for the two other surface families, {011} and {111}, in which the mirror symmetry of the crystal's rock-salt structure plays the same role. For {n n m} surfaces the four L-points in the 3-dimensional Brillouin zone project to four different points in the 2-dimensional Brillouin zone, but only when n and m have the same parity (it means of course that they are both odd numbers). When the parities of n and m are different, the L-points are projected in pairs. In this case, two protected Dirac points appear on the mirror symmetry line in the vicinity of the L-projection. Only for (001) surface there are two such lines and four Dirac points are topologically protected. Indeed, our calculations show that while in (111) $Pb_{0.4}Sn_{0.6}$ Te four single topologically protected Dirac-cones should appear, for the (011) surface states the protection is lifted for two L points projections. In this case, instead of the Dirac points energy gaps for the surface states occur, due to the interaction between the two L valleys. The spin polarization of metallic surface states in the TCI phase of $Pb_{0.4}Sn_{0.6}Te$ has been studied by calculating the in-plane spin texture along the constant-energy lines of the surface states. For all studied surfaces, (001), (011) and (111), chiral spin textures have been obtained. The research leading to these results has received funding from the European Community's 7th Framework Programme [FP7/2007-2013] under grant agreement n° 215368, the European Regional Development Fund through the Innovative Economy grant (POIG.01.01.02-00-108/09), and the Polish National Science Centre (NCN) Grant No. 2011/03/B/ST3/02659.

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P6. Dual effect of crowders on fibrillation kinetics of polypeptide chains revealed by lattice models

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We have developed the lattice model for describing polypeptide chains in the presence of crowders. The influence of crowding environment on the fibrillation kinetics of polypeptide chains is studied using this model. We observed the non-trivial behaviour of the fibril formation time that it decreases with the crowder concentration if crowder sizes are large enough, but the growth occurs for crowders of small sizes. This allows us to explain the recent experimental observation that for a fixed crowder concentration the fibril growth kinetics is fastest at intermediate values of total surface of crowders. It becomes slow at either small or large overages of cosolutes. It is shown that due to competition between the energetics and entropic effects the dependence of fibril formation time on the size of confined space is described by a parabolic function.

P7. In silico and in vitro characterization of anti-amyloidogenic activity of vitamin K3 analogues for Alzheimer's disease

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Because amyloid-beta (Aβ) aggregation may be the main cause of Alzheimer's disease (AD), and because the deficiency of Vitamin K has been exploired to be related to AD pathogenesis, in this study, we learned about the anti-amyloidogenic activity of 15 Vitamin K3 derivatives both in silico and in vitro. Biological and spectroscopic assays were used to characterize the effect of VK3 analogues on amyloidogenic properties of Aβ, such as aggregation, free radical formation, and cell viability. Molecular dynamics simulation was used to calculate the binding affinity and mode of VK3 analogue binding to Aβ. Both numerical and experimental results showed that several VK3 analogues could effectively inhibit A aggregation and conformational conversion. Among them, VK3-10, VK3-6, and VK3 have inhibition constants in the μM range, which is similar to that of curcumin. Moreover, VK3-9 could effectively reduce free radicals and had a protective effect on cytotoxicity induced by Aβ aggregates.

P8. Analysis of Binding Affinity of Protein-Ligand Complexes

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Binding of ligands such are Curcumin, Naproxen, Ibuprofen, 342 compounds derived fromVietnamese plants and 15 VK3 analogues to Aβ1−40 peptide and its fibrils is studied by docking method and all-atom molecular dynamics simulations. The binding mechanism is studied in detail showing that the van der Waals interaction between ligand and receptor dominates over the electrostatic interaction. The binding free energies obtained by the molecular mechanic-Poisson−Boltzmann surface area method indicate that some of them may be good candidates to cope with AD. Our results are in good agreement with the experiments.

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P9. Estimation of the Binding Free Energy of AC1NX476 to HIV-1 Protease Wild-Type and Mutations Using Free Energy Perturbation method

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The binding mechanism of AC1NX476 to HIV-1 protease wild-type and its mutations was studied by the docking and molecular dynamics simulations. The binding free energy was calculated by the double-annihilation binding-free energy method. The binding affinity of ritonavir to HIV-1 protease wild-type was also estimated for comparison with AC1NX476. Our theoretical results are in excellent agreeent with the experiment data as the correlation coefficient between calculated and experimentally measured binding free energies R = 0.994. The binding propensity is mainly driven by the van der Waal interaction, but a ligand with many negatively charged atoms would strongly block the activity of HIV-1 protease via the electrostatic interaction. The interaction between the ligand and receptor decreases with the number of water molecules that are non-bonded with the ligand. Residues Asp25, Asp29,Asp30, Ile47, Gly48, Val50, and Asp124 in the binding pocket play a crucial role in the ligand binding affinity. The mutation points belonging to the binding site were found to reduce the binding affinity by increasing its volume.

P10. Binding of fullerene to amyloid beta fibrils: Size matters

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Binding affinity of fullerenes C20, C36, C60, C70 and C84 to Aβ40 and Aβ42 fibrils is studied by docking and all-atom molecular dynamics simulations with the Amber 99SB force field and water model TIP3P. Using the molecular mechanic-Poisson Boltzmann surface area method for estimation of the binding free energy one can show that he larger is the fullerene size, the higher is binding affinity. Overall, fullerenes bind to Aβ40 fibrils stronger than to Aβ42 ones. The area between fibril layers is more dry than inside fibrils. Our study revealed that the van der Waals interaction dominates over the electrostatic interaction and non-polar residues play the significant role in interaction with fullerenes providing novel insight into the development of drug candidates against Alzheimer's disease.

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