WVSiP2017

Hội Thảo Sinh Viên toàn Ba lan lần thứ hai

Vác-xa-va, 23-24 tháng 9 năm 2017

Program and abstracts

Dear Colleagues and Friends,

We are glad to welcome you at the Second Workshop of Vietnamese Students in Poland (WVSiP2017) held in September 23-24, 2017 at the Institute of Physics, Polish Academy of Sciences in Warsaw.

The first edition of this workshop took place for the first time in Cracow in September 24-25, 2016. Beside of lectures presented by senior scientists, there were many interesting talks from our Ph.D. and M.Sc. students. We then decided that the workshop will be organized every year, each year in a different city. The workshop is open not only for Vietnamese graduates and postdocs in Poland but also for people from other countries.

The aim of the workshop is to offer an opportunity for participants to meet in an informal environment to discuss the latest advances in the field and to present their activities, to make connections and to initiate cooperation. The topics of the workshop are all domains of natural sciences, social sciences and technology.

The workshop is jointly organized by the Le Qui Don Society, Institute of Physics, Polish Academy of Sciences in Warsaw and Foundation for Supporting Integration of Vietnamese in Poland.

We wish you a fruitful and enjoyable time at the workshop and in Warsaw.

Organizers of WVSiP2017.

Các bạn và đồng nghiệp thân mến,

Nhiệt liệt chào đón các bạn tham dự Hội Thảo Sinh Viên toàn Ba lan lần thứ hai tổ chức ngày 23-24 tháng 9 năm 2017 tại Viện Vật Lý thuộc Viện Khoa Học Ba lan ở thành phố Vac-xa-va.

Hội thảo lần thứ nhất về chủ đề này đã được tổ chức ở thành phố Cra-côv ngày 24-25 tháng 9 năm 2016. Ngoài những bài giảng trình bày bởi những nhà khoa học có kinh nghiệm lâu năm, trong hội thảo có nhiều báo cáo rất lý thú do các nghiên cứu sinh và các sinh viên trình bày. Do đó, chúng tôi đã quyết định sẽ tổ chức hội thảo thường niên và mỗi năm sẽ chọn địa điểm khác nhau. Hội thảo không chỉ dành cho các sinh viên và những tiến sĩ trẻ Việt nam sau khi tốt nghiệp tại Ba Lan mà cả ở các nước khác tham dự.

Mục đích của hội thảo là tạo điều kiện cho những người tham dự cùng gặp gỡ trong khung cảnh thân mật để thảo luận về những tiến bộ mới nhất trong lĩnh vực nghiên cứu và trình bày các hoạt động khoa học của mình, để kết nối và mở hợp tác. Các chủ đề trong hội thảo bao gồm tất cả các lĩnh vực của khoa học tự nhiên, khoa học xã hội và công nghệ.

Hội thảo do câu lạc bộ Lê Quí Đôn, Viện Vật Lý Viện Khoa Học Ba lan và Quỹ hỗ trợ hội nhập của người Việt Nam tại Ba Lan phối hợp tổ chức.

Ban tổ chức hội thảo.

ORGANIZING COMMITTEE

Mai Suan Li, Institute of Physics, Polish Academy of Sciences, Warsaw (Chair)
Mariusz Gajda, Institute of Physics, Polish Academy of Sciences, Warsaw (Co-chair)
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Pham Dinh Quoc Huy, Institute of Physics, Polish Academy of Sciences, Warsaw

PLENARY and INVITED SPEAKERS

Łukasz Cywiński (Warsaw, ***plenary***)
Binh Khanh Mai (Sweden)
Hung Son Nguyen (Warsaw, ***plenary***)
Hoa Kim Ngan Nhu-Tarnawska (Krakow)
Adolfo Poma (Warsaw)
Zbigniew Tarnawski (Krakow)
Vinh Hung Tran (Wroclaw)
Yani Zhao (Warsaw)
Piotr Ziółkowski (Poznań, ***plenary***)

VENUE

Institute of Physics, Polish Academy of Sciences,
Al. Lotnikow 32/46, 02-668 Warsaw, Poland.
Building 1, the L. Sosnowski's auditorium.

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ABSTRACT BOOK EDITOR

Nhu-Tarnawska Hoa Kim Ngan

PROGRAM

Saturday, September 23, 2017		
8:00-9:00	Registration	
9:00-9:10	Opening Honored guests: Prof. Dr hab. **Grzegorz Grabecki**, Vice-Director of Institute of Physics, Polish Academy of Sciences (*GS TSKH, Viện phó Viện Vậy Lý, Viện Hàn Lâm Khoa Học Ba lan*) Mr. **Lê Thiết Hùng**, President of the Vietnamese Association in Poland (*Chủ tich Hội người Việt Nam tại Ba Lan*)	
9:10 - 9:50 **Pl-01**	Piotr A. Ziółkowski	From simple selection to genome editing and beyond
9:50-10:20 **I-01**	N.-T.H. Kim-Ngan	Hydrogen storage in metal hydrides: the case of U-based alloys with cubic structure
10:20-10:50	*Coffee/tea break*	
10:50-11:20 **I-02**	Z. Tarnawski	Superconducting phase transitions in mK temperature range:the experiments possibility by Triton in Krakow
11:20-11:40 **O-01**	Yongjie J. Wang	High pressure effect on structural and spectroscopic properties of Ce-doped $Y_4Al_2O_9$ single crystals
11:40-12:00 **O-02**	Thi Thu Ha Nguyen	High-T_c Superconductors: a new challenge for materials science
12:00-12:20 **O-03**	Mai Van Hai	Using EBSCOweb to search and write systematic review chapter of the dissertation
12:20-14:00	*Lunch*	
14:00-14:40 **Pl-02**	Łukasz Cywiński	Coherent control of quantum systems: from quantum computers to nanoscale sensors
14:40-15:10 **I-03**	Vinh Hung Tran	A very short introduction to density functional theory
15:10-15:30 **O-04**	Przemysław Kowalik	Multifunctional nanoconstructs based on up-converting rare-earth ions doped $NaYF_4$ and magnetic Fe_3O_4 nanoparticles for biological and medical applications
15:30-16:00	*Coffee/tea break*	

16:00-16:30 **I-04**	Adolfo Poma	GoMartini: Study of Large Conformational Transition in Proteins with the Martini Force-Field
16:30-16:50 **O-05**	Xuzhu Zhang	Tracking Structural Transitions of Bovine Serum Albumin in Surfactant Solutions by Fluorescence Correlation Spectroscopy and Fluorescence Lifetime Analysis
16:50-17:10 **O-06**	Nguyen Truong Co	Dual effect of crowders on fibrillation kinetics of polypeptide chains revealed by lattice models
17:10-17:30 **O-07**	Thanh Thuy Tran	Lattice model for amyloid-β peptides: OPEP force field parametrization and applications to the nucleus size of Alzheirmer's peptdies
19:00-21:30	*Conference dinner* *(Restaurant Lili, Al. Jerozolimskie 123 A, Warszawa)*	
Sunday, September 24, 2017		
9:00-9:40 **Pl-03**	Hung Son Nguyen	Data Science: challenges, directions and opportunities
9:40-10:10 **I-05**	Binh Khanh Mai	Theoretical Studies for Reaction Mechanism and Selectivity of Metal-Catalyzed Reactions
10:10-10:30	*Coffee/tea break*	
10:30 -11:00 **I-06**	Yani Zhao	Proteins at air-water and oil-water interfaces in an all-atom model
11:00-11:20 **O-08**	Łukasz Mioduszewski	Coarse-grained model of intrinsically disordered proteins
11:20-11:40 **O-09**	Hao Duong Van	3D model of the Sin Quyen copper deposit in Lao Cai province, North Vietnam
11:40-12:00 **O-10**	Dinh Quoc Huy Pham	Fullerenol $C_{60}(OH)_{16}$ prevents amyloid fibrillization of $A\beta_{40}$ – in vitro and in silico approach
12:00-12:10	Closing remarks	
12:10-13:00	*Lunch*	
13:00-18:00	Excursion (optional)	

Pl - plenary speaker **I - invited speaker**

ABSTRACTS

Pl-01

From simple selection to genome editing and beyond

Piotr A. Ziółkowski
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Recent advances in genome sequencing and engineering technologies open new exciting opportunities for generation of novel DNA variation and cellular function. These could be used to optimize food supply, increase production of bioenergy and chemicals, as well as improve environmental remediation. Most importantly, new strategies have a potential to treat human diseases and alleviate genetic disorders. I will present the state of the art in this field with a special focus on CRISPR-Cas9 technique, drawing also future directions for research and application perspectives. However, human efforts aiming to improve "natural" forms of life have a much longer history, therefore the new advances will be shown in the background of previous achievements. Extensive introduction for those students, who are not familiar with genetics and molecular biology, will be provided.

PI-02

Coherent control of quantum systems: from quantum computers to nanoscale sensors

Łukasz Cywiński
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Small quantum systems, such as spins of electrons localized in semiconductor nanostructures, can be used as building blocks of quantum computers.

I will try to explain the motivation for trying to build such computers, and the reasons for which this is a hard task. Luckily, even if turning a large number of spins into a quantum computer turns out to be prohibitively hard, there are other interesting things that can be accomplished when we have coherent control over small quantum systems. One of them is using single spins as sensors of fluctuations of local magnetic fields in nanoscale. This is a quickly developing field of research, with possible applications in chemistry and biology.

PI-03

Data Science: challenges, directions and opportunities

(Khoa học dữ liệu: thách thức, hướng đi và cơ hội)

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Data Scientist, according to users of online employment analysts Glassdoor, came out with the overall best score in the 2016 report. To many, it might seem surprising to pick data scientist as the “best job”. Sure, it is well paid and you get to tell people that your job is predicting the future – but is it really better than being an astronaut, professional athlete, or lead singer in a rock band?

The aim of this talk is to explain the reason of this phenomena and to convince the young students to consider it as one of the most interesting and most challenging disciplines in the era of Industry 4.0

The concept of data science was originally proposed within the statistics and mathematics community, where it essentially concerned data analysis. Data science today goes beyond specific areas like data mining and machine learning or whether it is the next generation of statistics. Formally, data science is a new trans-disciplinary field that builds on and synthesizes many relevant disciplines and bodies of knowledge, including statistics, informatics, computing, communication, management, and sociology, to study data following "data science thinking" (see Figure 1).

In this talk we plan to talk about the history and the main issues of data science and to present some typical applications of data science in our everyday life. We will have also a discussion about the two main challenges concerning the intrinsic complexities and intelligence in data science. We also consider the main research directions and application areas of data science in the nearest future. At the end, we will focus on the most important skills that potential data scientists must have to be competitive in this growing marketplace.

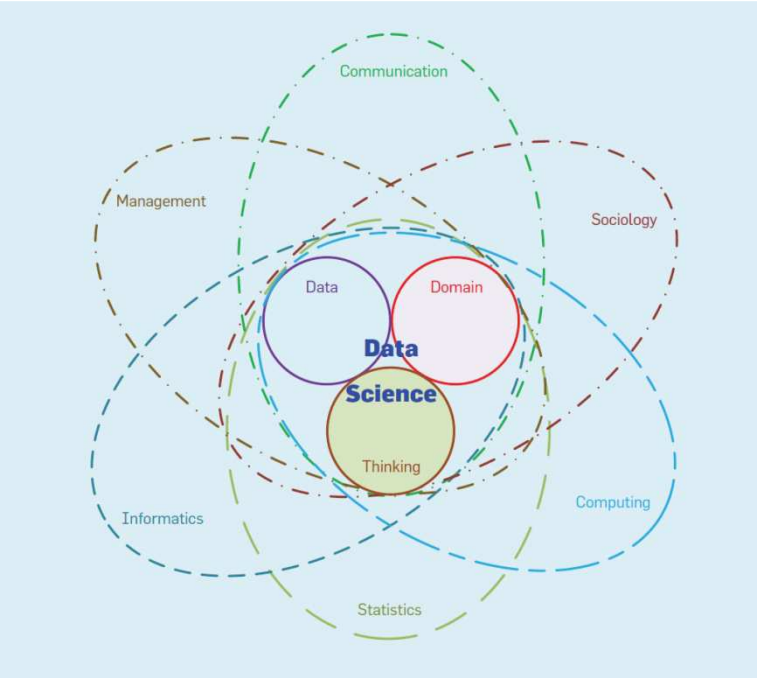

Figure 1. Data science = {statistics ∩ informatics ∩ computing ∩ communication ∩ sociology ∩ management | data ∩ domain ∩ thinking }

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[1] Longbing Cao. Data Science: Challenges and Directions. Communications of the ACM, Vol. 60 No. 8, Pages 59-68

[2] Tu Bao Ho. Khoa học dữ liệu trong cách mạng công nghiệp lần thứ tư

[3] Bernard Marr. Is Being A Data Scientist Really The Best Job In America? https://www.forbes.com/sites/bernardmarr/2016/02/25/is-being-a-data-scientist-really-the-best-job-in-america/

I-01

Hydrogen storage in metal hydrides: the case of U-based alloys with cubic structure

N.-T.H. Kim-Ngan[1,*], L. Havela[2], V. Buturlim[2], M. Paukov[2], S. Sowa[1], M. Krupska[1]

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(Hoa Kim Ngan NHU-TARNAWSKA)

Hydrogen and fuel cells are considered as key solutions for the 21st century, offering a clean and efficient production of power and heat especially without any negative impact on environment. Hydrogen storage is thus becoming a materials science challenge in developing hydrogen economy. One of the main goals is to search for optimal hydrogen-storage materials. Many metals and their alloys can absorb a large amount of hydrogen forming the so-called metal hydrides. Such systems with reversible hydrogen reaction are potential hydrogen storage media. The most widely utilized metal hydrides are MgH_2 and $LaNi_5H_6$. MgH_2 has a high storage capacities of hydrogen as much as 110 kg-H_2/m^3. The volumetric hydrogen density of $LaNi_5H_6$ is similar (115 kg-H_2/m^3). They are much higher than that of liquid hydrogen (70.85 kg-H_2/m^3 below 20 K) and hydrogen gas (0.09 kg-H_2/m^3 pressurized at 200 bar) [1]. Beside of volume-efficient storage, the advantage of metal hydrides is that they are stable and can be maintained at room temperature (while e.g. the liquid hydrogen has to be maintained at low temperature $T < 20$ K and the gas-hydrogen requires a large tank to store).

Our work concerns the hydrides of f-metals, such as Uranium. Metallic uranium consisting of the orthorhombic α-U phase (at and below the ambient temperature) strongly reacts to hydrogen at very low pressures (mbar), forming uranium-trihydride (UH_3) which is the only binary uranium hydride. UH_3 has two crystals structures: the metastable α-UH_3 phase formed at low temperatures which slowly converts to the stable β-UH_3 phase at high-temperatures. Both phases are cubic with similar crystal densities. UH_3 is a nasty pyrophoric powder which self-ignites in air and thus it is considered as a hazard during the storage of uranium metal.

The high-temperature body-centered cubic γ-U phase can be retained down to room temperature by alloying with transition metals (T). The alloys crystallizing in the cubic γ-U phase have a higher corrosion resistance and better

accommodate radiation damage (than those with α-U phase) and thus they are considered as better materials for nuclear fuels. Recently, we have succeeded in a stabilization of the cubic γ-U phase down to room temperature by alloying with Mo, Zr, Pt, Nb, Ru, Ti. All splat-cooled alloys consisted of pure γ-U phase are very stable in the air and ambient hydrogen atmosphere.

We have performed the hydrogenation experiments and underlined the hydrogen absorption ability in these splat-cooled alloys as well as hydrogen influence on the electromagnetic properties. Hydrogenation of $U_{1-x}T_x$ alloys consisted of γ-U phase leads to 3 different structures in the formed hydrides [2,3]. Using Zr alloying we succeed to synthesize the (crystalline) α-UH_3 phase as a pure phase without a transformation to β-UH_3. Using Mo alloying leads to a formation of the β-UH_3 phase in a new form-the nanocrystalline one. Using Ti alloying, we obtain a mixture of crystalline α-UH_3 and β-UH_3 in the hydrides with 10-15 at.% Ti, while those with higher Ti concentrations reveal the nanocrystalline β-UH_3 structure. The total amount of H_2 released corresponds to 2.7 H atoms per 1 U atom in all investigated hydrides. Thus we use generally the formula $(UH_3)_{1-x}T_x$. All γ-U alloys are weak Pauli paramagnets revealing superconductivity below 2.2 K [4]. The related hydrides $(UH_3)_{1-x}T_x$ are ferromagnets with much enhanced Curie temperatures T_C reaching even if 200 K. The uranium magnetic moment is of about $\mu_U = 0.9\mu_B$/U. Uranium magnetic moment is induced by hydrogen absorption as a result of a reduction of the 5*f* bandwidth and an increase of the density of state at the Fermi level due to a reduction in the overlap of the 5*f* wave functions between nearest U neighbors caused by a crystal structure expansion [5]. The crucial is that such hydrides are not pirophoric. Their handling and use are safe. It opens a possibility to use them for hydrogen storage applications. Besides, it is a very practical technique to produce the γ-U alloys in a powder form by a combination of hydrogenation, followed by crushing of the brittle hydrides into powders and then by hydrogen desorption (of the powders) in a vacuum.

This work was supported by the Czech Science Foundation (Grant 15-01100S). Experiments were partly performed at MLTL (http://mltl.eu/) supported within the program of Czech Research Infrastructures (project No. LM2011025).

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[2] I. Tkach et al., Phys. Rev. B 88 (2013) 060407R.
[3] I. Tkach et al., Phys. Rev. B 91 (2015) 115116.
[4] N.-T.H. Kim-Ngan et al., J. Nuclear Materials 479 (2016) 287-294.
[5] L. Havela, N.-T.H. Kim-Ngan, Adv. Nat. Sci.: Nanosci. Nanotechnol. 8 (2017) 015005.

I-02

Superconducting phase transitions in mK temperature range: the experiments possibility by Triton in Krakow

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We present the temperature and magnetic-field dependence of the electrical resistivity (ρ (T,B) dependence) for selected $U_{1-x}T_x$ alloys (T= Pt, Ti, Ru, $x \leq 0.30$) prepared by splat-cooling technique. The measurements were carried out by means of Triton ^{3}He/^{4}He dry dilution refrigerator allowing to collect the data down to 10 mK in magnetic files 0 - 14T, which are highly required for constructing the H-T diagram, since the investigated materials revealed the critical temperatures below 400 mK-the temperature limit of Quantum Design Physical Properties Measurement System (PPMS).

In most of investigated alloys, a single resistivity drop was observed at the superconducting transition, while the splat-cooled $U_{0.85}Pt_{0.15}$ alloys exhibit two superconducting transitions denoted as T_c (the main transition) and T_c^* (the additional transition) for which the characteristics of the ρ(T,B) curves revealing a dependence on the cooling rate during sample preparation. The measurements performed on several different splats with the splat-thickness d < 150 μm (the splat-cooled disc-shape samples prepared from a sample ingot with a mass < 300 mg and with the proper cooling rate of 10^6 K/s during sample preparation) revealed the main drop at T_c = 0.95 K (with the transition width ΔT_ρ = 0.06 K) and the additional drop at T_c^*=0.61 K. A thicker splat (with a disc-shape prepared from a bigger sample ingot) with $d \approx$180 μm shows an opposite pattern, i.e. the main drop T_c= 0.61 K (with ΔT_ρ = 0.04 K) and a minor additional drop at and T_c^* = 0.95 K. The $\rho(T)$ dependence of the drop-like splat as a consequence of a much slower cooling rate than 10^6K/s) revealed three features, namely the smooth decrease from 1.0 K to 0.8 K (in which the resistivity value decreases by 50%), followed by a plateau in the temperature range of 0.8 - 0.6 K and an abrupt drop below 0.6 K (in which the relative resistivity value decreases by 40%). In this

case, the transition temperature determined at the half height of the resistivity are denoted as T_c (high) and T_c (low), respectively, appearing at 0.9 K (with ΔT_ρ = 0.20 K) and 0.58 K (with ΔT_ρ = 0.05 K).

The temperature dependence of the upper critical fields H_{c2} in the *H-T* phase diagram is quite similar for all investigated splats and in a good agreement with the Ginzburg-Landau approximation. The estimated values for the critical magnetic field at 0 K ($\mu_0 H_{c2}$ (0)) and the critical slopes at T_c of the H_{c2} vs T curves($-\mu_0(dH_{c2}/dT)_{Tc}$) are in the range of 1 - 5 T and 2 - 4 T/K respectively. No λ-type anomaly was observed in the specific heat. The specific-heat jump at T_c is much smaller than that estimated from BCS theory.

I-03

A very short introduction to density functional theory

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Computational approaches play an important role in various branches of modern sciences as they not only help us to better understand complex and diverse phenomena, e.g., from living systems to exotic ground states of condensed matter, but also allow us to discover and design new useful materials. In this talk, I will try to introduce young scientists to scientific concepts of density-functional theory (DFT) through explanation of some essential basics and discussing several topics beyond DFT. *I shall start* with definitions of a few terms used in DFT, and then I will give an overview concerning a couple of most applicable methods for numerical simulation in computational sciences. *In the next part of my talk*, I will focus on full-potential methods which have been used by me on doing electronic band structure calculations for magnetic and superconducting compounds. For illustration, one of results of DFT calculations for superconducting Th_7Fe_3 is presented in Fig. 1, where there are 3D- crystal structure and electron localization function (ELF) representations cutting (a), in the (001)- (b), (010)- (c) and (110)-plane (d), respectively.

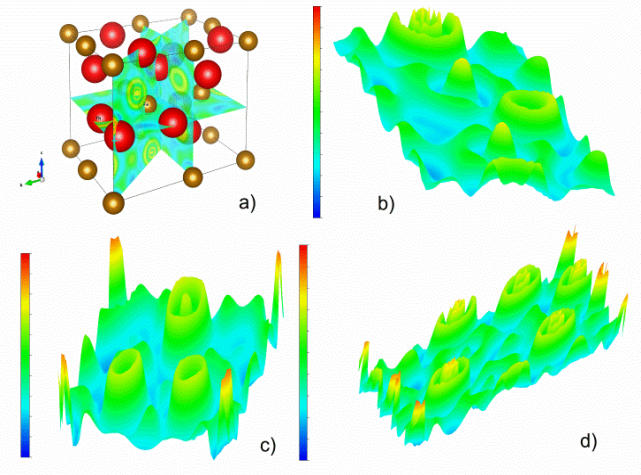

Fig. 1. 3D vizualizations of crystal unit cell of superconducting Th_7Fe_3 and the ELF iso-surfaces cutting (a), in the b) (001)-plane, c) (010)-plane and d) (110)-plane, respectively. The ELF values are bound between 0 (blue color) and 1 (red color). The data predict the electron density distribution, types of bonds and their properties in the crystal of the investigated compound.

Furthermore, in short, I will notify possible troubles during compilation of source codes and limitations that may arise out of software being used. *Finally*, I will provide useful links to selected DFT based electronic structure codes together with brief comments for them.

I-04

GoMartini: Study of Large Conformational Transition in Proteins with the Martini Force-Field

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The application of Coarse-Grained (CG) models in biology is essential to access large length and time scales needed for the description of several biological processes (e.g. self-assembly of beta-peptides into disease/functional amyloid fibrils, dissociation of protein-protein complexes, large movement of proteins under high mechanical stress, etc). The ELNEDIN [1] protein model is based on the well-known MARTINI CG force-field and incorporates additionally "harmonic bonds" of a certain spring constant within a defined cutoff distance between pairs of amino acid residues, in order to retain the native structure of the protein. In this case, the use of unbreakable harmonic bonds hinders the study of unfolding and folding processes. To overcome this barrier we have replaced the harmonic bonds with Lennard–Jones interactions based on the contact map of the native protein structure as is done in Go-like models. Our model [2] (see Figure 1) exhibits very good agreement with all-atom and the ELNEDIN simulations. Furthermore, our model is based on the van der Waals radii, instead of a cutoff distance, which results in a smaller number of interactions compared to ELNEDIN model. In conclusion, we anticipate that our model will provide further possibilities for studying biological systems beyond the scope of the ELNEDIN protein model.

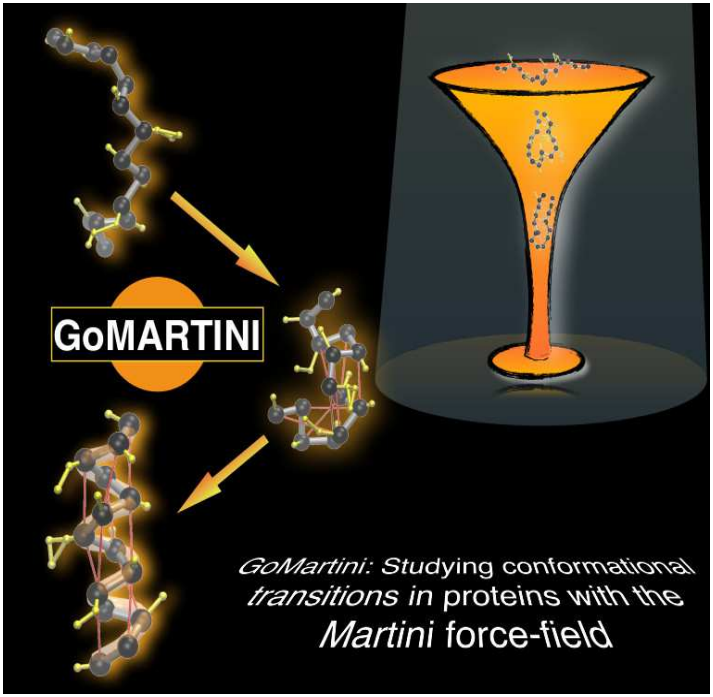

Figure 1. Schematic representation of the folding process for an α-helix using the GoMartini model.

References

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I-05

Theoretical Studies for Reaction Mechanism and Selectivity of Metal-Catalyzed Reactions

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Computational chemistry has become an essential tool for all branches of chemistry, in particular for organic and organometallic chemistry.

In our works, we are interested in applying computational methods (density functional theory calculations) to understand mechanistic insights into metal-catalyzed reactions, focusing on reactivity and selectivity. Our researches are in close collaboration with experimental works to explain experimental results and develop new efficient catalysts.

In this presentation, I will summarize some of our computational studies for metal-catalyzed reaction mechanism.

I-06

Proteins at air-water and oil-water interfaces in an all-atom model

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We study the behavior of five proteins at the air-water and oil-water interfaces by all-atom molecular dynamics. The proteins are found to get distorted when pinned to the interface. This behavior is consistent with the phenomenological way of introducing the interfaces in a coarse-grained model through a force that depends on the hydropathy indices of the residues. Proteins couple to the oil-water interface stronger than to the air- water one. They diffuse slower at the oil-water interface but do not depin from it, whereas depinning events are observed at the other interface. The reduction of the disulfide bonds slows the diffusion down.

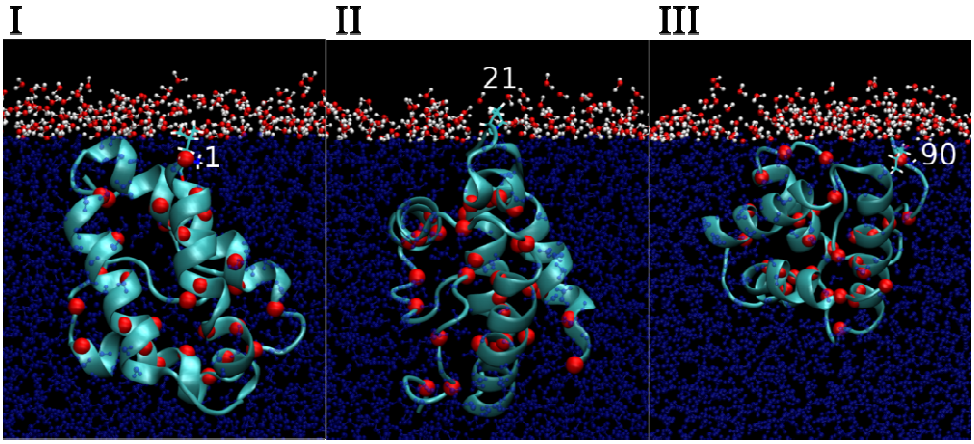

Fig 1. Three adsorption pathways of protein 1LIP to the air-water interface.

References

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O-01

High pressure effect on structural and spectroscopic properties of Ce-doped $Y_4Al_2O_9$ single crystals

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YAM:Ce single crystals with various concentrations up to 1% of Ce, grown by micro-pulling down (μ-PD) method were studied in this work. The structure of YAM has been accurately determined from single-crystal X-ray diffraction (XRD) data. The obtained crystals were characterized by various spectroscopic techniques, such as FT-IR, absorption, Raman, luminescence, photoluminescence excitation, etc.

Efficient luminescence of this material, which appears in a blue spectral region between 430 and 540 nm, undergoes strong temperature quenching, which begins already at temperature of about 20 K. The luminescence quenching is thermally activated with activation energy equal to ~ 21 meV.

We associate this quenching with position of the 5d state of Ce^{3+} close to the bottom of the conduction band[1]. High pressure luminescence experiments, performed in diamond anvil cell confirm this hypothesis. Due to pressure induced increase of the separation energy between the 5d states of Ce3+ ions and a bottom of the conduction band the temperature of the luminescence quenching is increased. Furthermore, It was found that Ce^{3+} luminescence reveals an abrupt red shift at pressure of above 10 GPa, which might be a fingerprint of phase transition. Evidence of phase transitions of YAM under high pressure was obtained using angular dispersive synchrotron X-ray diffraction (ADXD) and Raman spectroscopy. The results of XRD , Rman spectra and PL are in fairly good agreement with each other.

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O-02

High-T_c Superconductors: a new challenge for materials science

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Superconductivity is a phenomenon which occurs in some materials and can be characterized by zero electrical resistance, complete ejection of magnetic fields from the inner part of sample and Josephson effects. The phenomenon was first discovered by Onnes in the year 1911, when he cooled the mercury below 4.2 K [1]. Owing to unique electrical, magnetic and quantum mechanical properties, superconductors result in many useful applications in both basic research and industrial technology. High magnetic field electromagnets, SQUID devices, MRI and levitating trains are just a few examples.

The discovery of superconductivity in copper-oxide compounds by Bednorz and Müller in 1986 [2] has opened new perspectives for superconducting materials science, since the critical temperature T_c is reached until today up to 135 K and upper critical field H_{c2} even up to 45 T. Iron-based superconductors discovered in the year 2008 by Kamihara et al. [3] are next newcomers of the high-T_c superconductors family and obviously this discover raises new challenge of researches. It is not only searching for superconducting materials with higher T_c and H_{c2} but also finding answer the question of how do high-T_c superconductors work? In order to explore the underlying mechanism for high-T_c superconductivity, it is necessary to determine the physical properties, simultaneously at the macroscopic and at microscopic levels. My master thesis concerns the issue of coexistence of magnetism and superconductivity in the series of compounds $Sr_2MFeAsO_3$ (M = Sc, Ti, V, Cr), which were reported to have a short range magnetic transition at about 150 K and superconductivity at 37 K [4]. We plan to synthesize and carry out measurements of the bulk physical properties and Mössbauer spectra at low temperatures.

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O-03

Using EBSCOweb to search and write systematic review chapter of the dissertation

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University of Lodz, Poland.

EBSCOweb is library online that provides to researchers all information such journals, books in around the world.

This presentation will introduce how to use literatures from EBSCOwebs (search, collect, classify, etc literatures) to write the chapter of systematic review of a study.

This presentation will be useful for researchers in approach, search literatures those related to their study issues. Understanding this methodology/database is also useful to students, Ph.D students in process of researching and writing their result study.

O-04

Multifunctional nanoconstructs based on up-converting rare-earth ions doped $NaYF_4$ and magnetic Fe_3O_4 nanoparticles for biological and medical applications

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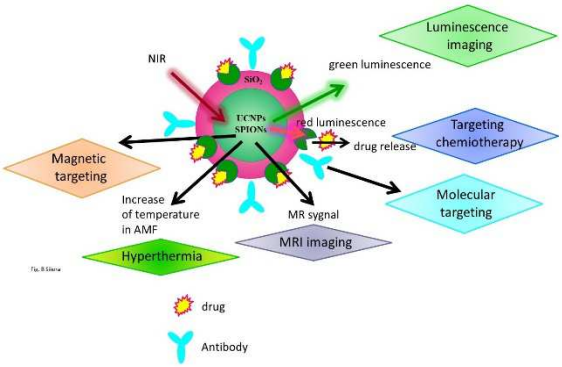
The main aim of our research was to create multifunctional system based on connecting of two types of nanoparticles – $NaYF_4$ nanocrystals with up-converting properties and Fe_3O_4 nanoparticles with superparamagnetic properties. The proposed system allows to prepare nanomaterials for theranostic applications (diagnostics and therapeutics). First of them, using near-infrared light as a excitation source, has potentially huge applications in biological studies because of relatively low absorption by water, low scattering and low autofluorescence level of organic components in this region. Second type of material – iron oxide nanoparticles – is suitable for magnetic hyperthermia. Superparamagnetic nanoparticles, exposed to alternating magnetic field, generate heat thus lead to damage of cellular membrane.. Coating of the above materials in a single silicon oxide shell further expands possibility for their surface modification thus generation of biologically specific, multitask materials.



NIR - near infrared (excitation light for UCNPs)
UCNPs - upconversion nanophosphors $NaYF_4$
SPIONs - superparamagnetic iron oxide nanoparticles Fe_3O_4
PDT – photodynamic therapy
MR – magnetic Resonance
AMF - alternating magnetic field

Reference

[1] P. Kowalik et al., RSC Adv., 2017,7, 30262-30273.

O-05

Tracking Structural Transitions of Bovine Serum Albumin in Surfactant Solutions by Fluorescence Correlation Spectroscopy and Fluorescence Lifetime Analysis

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We investigated the structural property of bovine serum albumin (BSA) in low concentrated cationic (cetyltrimethylammonium chloride, CTAC), anionic (sodium dodecyl sulfate, SDS), and nonionic (pentaethylene glycol monododecyl ether, $C_{12}E_5$ and octaethylene glycol monododecyl ether, $C_{12}E_8$) surfactant solutions by fluorescence correlation spectroscopy (FCS) and fluorescence lifetime analysis. We observed sudden structural transitions of BSA in SDS and CTAC solutions at the concentrations well below CMC, while no change was observed in the nonionic surfactant solutions. Therefore, the structural transition of BSA was induced by BSA/surfactant interaction but not by micelles. Moreover, by using FCS we are also able to identify whether the structural change of protein results from its self-aggregation or unfolding.

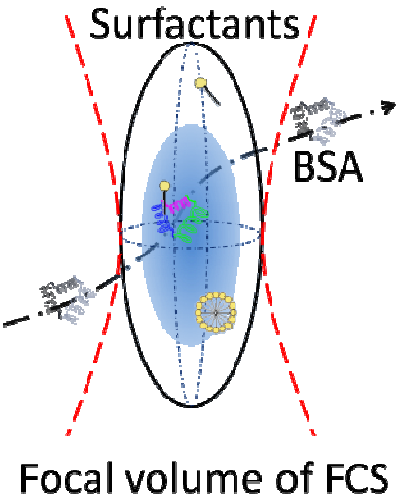

Fig. 1: BSA-Surfactant interaction within the focal volume of FCS

Reference

[1] X. Zhang et al., *Soft Matter*, 2015, 11, 2512.

O-06

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

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Neurodegenerative pathologies such as Huntington's Alzheimer's, Parkinson's, and prion diseases are associated with formation of amyloid oligomers and fibrils that have crossβ-sheet structure. Understanding mechanisms governing fibrillation kinetics of peptides and proteins plays a key role in finding out the way for their effective treatment. So far most of investigation has been focused on exploring kinetics of oligomerization in ideal homogeneous milieu. However, all living processes take place in crowded environment which comprises DNA, protein, lipid, and sugar occupying 20%–30% volume of the typical cell cytoplasm. Therefore this factor should be taken into account.

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

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[1] M. S. Li, D. K. Klimov, J. E. Straub, and D. Thirumalai, J. Chem. Phys.129, 175101 (2008)
[2] M. S. Li, N. T. Co, C. K. Hu, J. E. Straub, and D. Thirumalai, Phys. Rev. Lett.105, 218101 (2010)
[3] Nguyen Truong Co, Chin-Kun Hu, and Mai Suan Li, Dual effect of crowders on fibrillation kinetics of polypeptide chains revealed by lattice models, J. Chem. Phys. 138, 185101 (2013)

O-07

Lattice model for amyloid-β peptides: OPEP force field parametrization and applications to the nucleus size of Alzheirmer's peptdies

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The neurodegenerative Alzheimer's disease (AD) is affecting more than 40 million people worldwide and is linked to the aggregation of the amyloid-β proteins of 40/42 amino acids. Despite extensive experimental studies, the mechanism of formation of amyloid fibrils and plaques is still unclear. To complement experiments, computational studies based on all-atom simulations are very often used. They are however limited in the sampling problem for small systems and short time scales (ns-μs).

Protein lattice models approximate atomistic details and keep the essential interactions, but their force field is not optimal. Our primary aim is to develop a coarse-grained protein lattice model for amyloid proteins. This allows us to determine structures, thermodynamics and dynamics of very large amyloid systems, with the focus on the characterization of oligomers prior to nucleation, and the mechanisms leading to amyloid fibril.

In this talk, I will present a comprehensive OPEP force-field parameterization for two representative peptide fragments $(A\beta)_{16\text{-}22}$ and $(A\beta)_{37\text{-}42}$ of the Alzheimer's peptide (Aβ) using an on-lattice protein model, which incorporates explicitly the formation of hydrogen bonds and directions of side-chains with Monte Carlo simulations. Our bottom-up approach starts with the determination of the best force-field for the $(A\beta)_{16\text{-}22}$ dimer by fitting its equilibrium parallel and anti-parallel β-sheet populations obtained from the lattice simulations to that of all-atom simulations. Interestingly, the calibrated force-field is transferable to the trimer $(A\beta)_{16\text{-}22}$ as well as $(A\beta)_{37\text{-}42}$ dimer and trimer. Encouraged by this finding, we study the free energy landscapes of the two decamers. Our results show that the dominant structure of the $(A\beta)_{16\text{-}22}$ decamers is agreed with the microcrystal structure. Pushing the simulations for aggregates between 4-mer and 12-mer suggests a nuclues size for fibril formation of 10 chains [1]. In contrast, the decamers $(A\beta)_{37\text{-}42}$ is largely disorder with mixed by parallel and antiparallel chains, suggesting that the nucleus size is larger than 10 chains. Additional simulations for aggregation of $(A\beta)_{37\text{-}42}$ between 15 and 40

chains indicate a nucleus size is in order of 40 peptides [2,3]. Our refined force field coupled to this on-lattice model should provide useful insights into the critical nucleation number associated with neurodegenerative diseases.

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[1] T. T. Tran, P. H. Nguyen, and P. Derreumaux, J. Chem. Phys. **144**, 205103 (2016).

[2] M. Chiricotto, T. T. Tran, P. H. Nguyen, S. Melchionna, F. Sterpone, and P. Derreumaux, Israel Jounal of Chemistry, p. 10.1002/ijch.201600048 (2016).

[3] F. Sterpone, S. Doutreligne, T. T. Tran, M. Baaden, S. Melchionna, P. H. Nguyen, P. Derreumaux, accepted in Biochemical and Biophysical Research Communications (2017).

O-08
Coarse-grained model of intrinsically disordered proteins

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Intrinsically disordered proteins (IDPs) do not have one clearly defined structure and can adopt different conformations, depending on their environment. Therefore, a model of an IDP cannot be fully structure-based [1]. However, it can rely on statistical properties of a conformational ensemble of IDPs, obtained from all-atom simulations or experiment. I will present such a model, where one pseudo-atom represents one amino acid, local interactions (between pseudo-atoms adjacent in the protein chain) are based on random coil library [2], and nonlocal interactions (between pseudo-atoms not close to others in the chain) are modeled either by Lenard-Jones potential, similar to that used in the structure-based model [3] or by screened electrostatic potential for charged amino acids.

Our model was parameterized using a mix of experimental and all-atom simulation data for homopolymers, which are IDPs. Among them polyglutamine was given special attention, because polyglutamine tracts in some proteins are responsible for various neurodegenerative diseases and are known to aggregate into amyloids [4].

The model was also used to model gluten, a set of IDPs from wheat grains, responsible for dough elasticity and rich in glutamine [5].

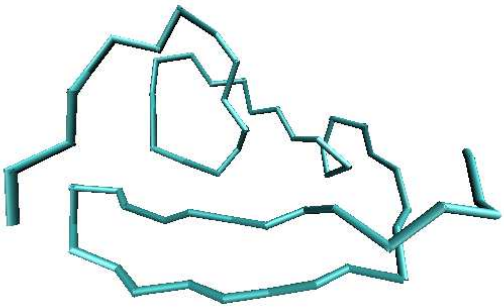

Fig. 1. One of modeled polyglutamine structures

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O-09

3D model of the Sin Quyen copper deposit in Lao Cai province, North Vietnam

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The Sin Quyen copper deposit located in Lao Cai province (North Vietnam) is the biggest copper deposit in Vietnam. The deposit is classified as the iron oxide copper gold (IOCG) deposit and has been being exploited since 2006 year. Using the "MineScape 5.12™" software and the geological data recorded from 146 boreholes, 21 tunnels and 216 outcrops, the 3D model of ore bodies was build. Recent data obtained from mineral and chemical analyses of 50 rock samples collected in 2014 and 2015 were incorporated into the model. The modeling process was principally consisted of four steps: the first is to set up the data, verify and store them in the consistent database; the second is to create the geometry of the ore bodies and estimate chemical parameters (grade) within the ore bodies; the third step is building of the horizontal and vertical sections using the verified and interpolated data and compare the results with data from database (Fig.1). The 3D model of ore bodies in the IOCG Sin Quyen deposit is shown in Fig.2. Based on the 3D model the copper resources in the deposit were estimated at 550000 Mg.

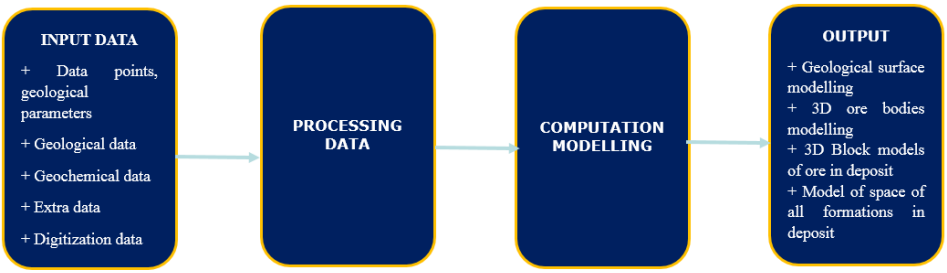

Fig.1. The schema of the 3D modelling process.

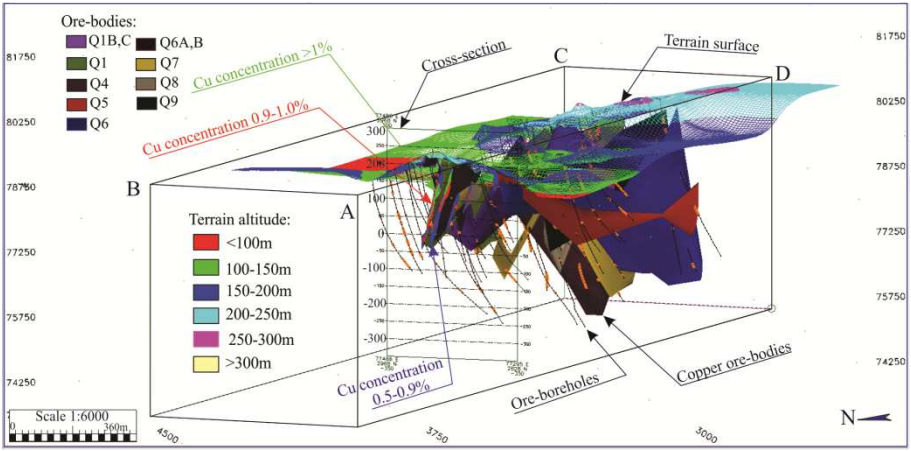

Fig.2. The 3D model of ore bodies in the IOCG Sin Quyen deposit.

O-10

Fullerenol $C_{60}(OH)_{16}$ prevents amyloid fibrillization of $A\beta_{40}$ – *in vitro* and *in silico* approach

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*Email: masli@if.pan.pl

The generation of Aβ amyloid aggregates in the form of senile plaques in the brain is one of the pathological hallmarks of Alzheimer's disease (AD). There is no cure for AD and one of the recent treatment strategies is focused on the inhibition of amyloid fibrillization of Aβ peptide. Fullerene C_{60} has been proposed as a candidate for destroying Aβ aggregates but it is not soluble in water and its toxicity to cells remains largely ambiguous. To overcome these drawbacks, we synthesized and studied the effect of water-soluble fullerenol $C_{60}(OH)_{16}$ (fullerene C_{60} carrying 16 hydroxyl groups) on the amyloid fibrillization of $A\beta_{40}$ peptide in vitro. Using a Thioflavin T fluorescent assay and atomic force microscopy it was found that $C_{60}(OH)_{16}$ effectively reduces the formation of amyloid fibrils. The IC_{50} value is in the low range ($\mu g.ml^{-1}$) suggesting that fullerenol interferes with $A\beta_{40}$ aggregation at stoichiometric concentrations. The *in silico* calculations supported the experimental data. It was revealed that fullerenol tightly binds to monomer $A\beta_{40}$ and polar, negatively charged amino acids play a key role. Electrostatic interactions dominantly contribute to the binding propensity via interaction of the oxygen atoms from the COO^- groups of side chains of polar, negatively charged amino acids with the OH groups of fullerenol. This stabilizes contact with either the D23 or K28 of the salt bridge. Due to the lack of a well-defined binding pocket fullerenol is also inclined to locate near the central hydrophobic region of $A\beta_{40}$ and can bind to the hydrophobic C-terminal of the peptide. Upon fullerenol binding the salt bridge becomes flexible, inhibiting Aβ aggregation. In order to assess the toxicity of fullerenol, we found that exposure of neuroblastoma SH-SY5Y cells to fullerenol caused no significant changes in viability after 24 h of treatment. These results suggest that fullerenol $C_{60}(OH)_{16}$ represents a promising candidate as a therapeutic for Alzheimer's disease.

References

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Information about the first edition of Workshop of Vietnamese Students in Poland in Cracow, September 24-25, 2016

http://info.ifpan.edu.pl/~masli/VietnameseStudentInPoland/index.html

http://info.ifpan.edu.pl/~masli/VietnameseStudentInPoland/index.html

Dear Colleagues and Friends,

We would like to invite you to attend The First Workshop of Vietnamese Students in Poland which will be held in Krakow on September 24-25, 2016. The aim of the workshop is to offer an opportunity for Vietnamese graduates and postdocs in Poland to meet in an informal environment to discuss the latest advances in the field, to present their activities, to make connections, and to initiate cooperation. The topics will be covered are all domains of natural and social sciences, and technology. The workshop is jointly organized by the Le Qui Don Society and Foundation for Supporting Integration of Vietnamese in Poland.

Best regards

Organizers

Venue

AGH University of Science and Technology

Faculty of Physics and Applied Computer Science

Al. Mickiewicza 30, 30-059 Kraków

Building C1, Lecture room 224.

Saturday, 24 September, 2016

9:00 - 10:00 Reception

10:00 - 10:10 Opening

10:10 - 10:50 **Hoa Kim Ngan Nhu-Tarnawska**, How to prepare a scientific paper?

10:50 – 11:10 **Mai Van Hai** , Gender equality in family relations of Vietnamese living in Vietnam and Poland.

11:10 – 11:30 *Coffee break.*

11:30 - 11:50 **Nguyen Truong Co**, Coarse-grained modeling of biosystems.

11:50 - 12:10 **Nguyen Viet Thanh**, Systems with hidden attractors.

12:10 - 12:30 **Duong Van Hao**, 3D Geochemical block modeling of the IOCG SinQuyen Deposit, North VietNam: Implication for resources evaluation.

12:30 - 14:00 *Lunch. Restaurant Lunch-Café, Reymonta 15.*

14:00 – 14:20 **Viet Ba Mai and Tymofiy Sichkar**, Music analysis module in a multiplatform game.

14:20 – 14:45 **Vo Van Thiep** , The growth characterisrics of fish species-Gerres filamentosus (Cuvier, 1829) in coastal zone, Quang Binh province.

14:45 – 15:10 **Pham Dinh Quoc Huy**, The effects of fullerenes on amyloid beta fibril.

15:10 – 15:30 *Coffee break*

15:30 – 16:00 **Dang Ngoc Han**, Paracel and Spratly Islands.

16:00 – 16:30 **G. La Penna**, Ions and disordered proteins.

16:30 – 17:00 **Nguyen Dinh Chau**, Scientific collaboration between Vietnam and Poland.

18:00 – 23: 00 *Workshop dinner, Starej Kuchnia" restaurant (Tomasza 8, the Market Square).*

Sunday, 25 September, 2016

9:00 - Sightseeing, trip to the saltmine Wieliczka

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Thông báo: Hội Thảo Sinh Viên Việt Nam tại Ba Lan

Nhằm mục đích tạo cơ hội cho sinh viên, nghiên cứu sinh và thực tập sinh Việt Nam tại Ba Lan gặp gỡ trao đổi kinh nghiệm học tập, nghiên cứu và hợp tác, các em sẽ được học hỏi thêm kinh nghiệm nghiên cứu từ các nhà khoa học đi trước đang làm việc tại các trường Đại học, cơ sở nghiên cứu ở Ba Lan, Câu lạc bộ Lê Quý Đôn cùng với sự tham gia của "Quỹ hỗ trợ người Việt Nam hội nhập tại Ba Lan" sẽ tổ chức **HỘI THẢO SINH VIÊN VIỆT NAM TẠI BA LAN**

Thời gian: Khai mạc vào lúc 10:00 , thứ Bảy, ngày 24/9/2016

Địa điểm: Khoa Vật lý và Tin học Ứng dụng, Đại Học Khoa Học và Công nghệ AGH Krakow mang tên Stanislaw Staszic, al. Mickiewicza 30, 30-059 Krakow

Xin trân trọng kính mời những ai quan tâm đến tham dự hội thảo

Sự có mặt của Quí vị là đóng góp quí báu cho thành công của Hội thảo.

Rất hân hạnh được đón tiếp Quý vị!

Warszawa, 10 tháng 9 2016

TM BTC

GS.TSKH. Mai Xuân Lý

Chủ tịch CLB Lê Quý Đôn tại Ba Lan

(Thông báo này thay cho giấy mời)

Chương trình Hội thảo

Ngày thứ nhất: 24/9

10:00-10:15 Khai mạc Hội thảo

10:15-12:30 Báo cáo khoa học

12:30-14:00 Ăn trưa

14:00-17:00 Báo cáo khoa học
18:30-23:00 Tiệc hội thảo
Ngày thứ hai, 25/9
Từ 9:00- Tham quan Krakow, mỏ muối Wieliczka
Chương trình chi tiết được đăng trên website của CLB Lê Quí Đôn tại Ba Lan (lequydon.org)

http://queviet.eu/gioi-tre/giang-duong/116106-hoi-thao-lan-thu-i-danh-cho-sinh-vien-nghien-cuu-sinh-viet-nam-dang-hoc-tap-nghien-cuu-tai-ba-lan
2016-09-26 10:58:53

Hội thảo lần thứ I dành cho sinh viên, nghiên cứu sinh Việt Nam đang học tập, nghiên cứu tại Ba Lan

GS.TSKH Mai Xuân Lý phát biểu khai mạc Hội thảo

Vào ngày 24/09/2016, tại Trường Đại học Khoa học và Công nghệ AGH, Krakow, CLB Lê Quý Đôn của các trí thức người Việt Nam đang làm việc, nghiên cứu và giảng dạy tại Ba Lan cùng với "Quỹ hỗ trợ người Việt Nam hội nhập tại Ba Lan" đã tổ chức thành công tốt đẹp buổi hội thảo dành cho các sinh viên, nghiên cứu sinh Việt Nam tại Ba Lan.

Có mặt và tham dự buổi hội thảo, bên cạnh các thầy cô là các giáo sư người Việt Nam đang giảng dạy, nghiên cứu tại Ba Lan còn có sự góp mặt của GS. Bartłomiej Szafran, Phó trưởng khoa Khoa Vật lý và Ứng dụng Khoa học Máy tính AGH, GS. Zbigniew Tarnawski - Trưởng khoa Vật lý Khoa rắn Vật lý và Khoa học ứng dụng máy tính AGH, bài tham luận của GS. Giovanni La Penna, Viện hợp chất hóa học hữu cơ kim loại (Florence, Italia).

Buổi hội thảo đã diễn ra trong vòng một ngày với 9 báo cáo của giáo sư, nghiên cứu sinh và sinh viên. Nội dung của các báo cáo tại hội thảo chủ yếu về mặt phương pháp luận như phương pháp viết bài tạp chí khoa học, sự hợp tác trong đào tạo giữa Việt Nam và Ba Lan, đề cương và kết quả bước đầu các

nghiên cứu của nghiên cứu sinh… Thông qua đó, mọi người có thể tham gia góp ý, chia sẻ những kinh nghiệm, lưu ý cho các bạn nghiên cứu sinh, sinh viên, tránh đi những sai sót trong quá trình học tập, nghiên cứu của mình.

Thực tế quá trình học tập của các nghiên cứu sinh, sinh viên Việt Nam tại Ba Lan đã chỉ ra bên cạnh những khó khăn về ngôn ngữ, các bạn trẻ cũng gặp không ít khó khăn do yêu cầu nghiêm khắc, khách quan của quá trình học tập, sự bị động do không quen với chương trình, cách thức đào tạo tại đây. Thậm chí nhiều người học hoàn toàn mơ hồ về những việc mình phải làm, các thủ tục phải giải quyết… trong quá trình học tập. Vì vậy, chương trình hội thảo do CLB Lê Quý Đôn tổ chức đã thực sự hữu ích, ý nghĩa đối với các nghiên cứu sinh, sinh viên. Sự chân thành, gần gũi giữa thầy và trò, giữa các giáo sư với nghiên cứu sinh… đã đem lại cho các bạn trẻ sự tự tin trong quá trình học tập, khuyến khích tình yêu khoa học đối với thế hệ trẻ. Các bạn cũng luôn mong muốn CLB Lê Quý Đôn tiếp tục tổ chức các hoạt động mang tính học thuật, tạo sân chơi khoa học để mọi người có điều kiện được cọ xát, học hỏi nhiều hơn nữa. Bên cạnh đó, các bạn trẻ cũng luôn bày tỏ sự tri ơn sâu sắc đến các thầy cô trong CLB Lê Quý Đôn, đặc biệt là sự tâm huyết của các GS.TSKH Mai Xuân Lý, GS.TSKH Nguyễn Đình Châu, GS.TSKH Nhữ Hoa Kim Ngân trong suốt quá trình chuẩn bị, triển khai hội thảo.

Một số hình ảnh trong hội thảo:

Các tài liệu cho hội thảo

Đại diện lãnh đạo trường AGH phát biểu tại hội thảo

Ảnh kỷ niệm cùng các GS quốc tế tham gia chương trình

Một số báo cáo viên trong HT

Trao đổi trong giờ giải lao

Bữa tối sau hội thảo

Tin và ảnh: MVH