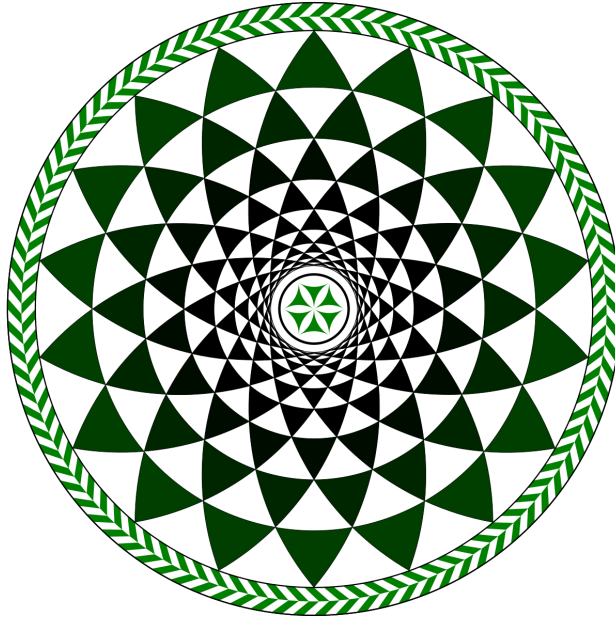


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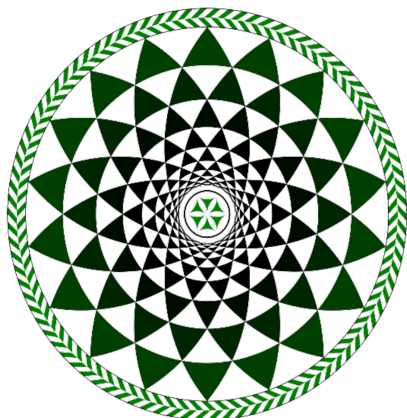
Multiscale phenomena in molecular matter

Kraków, 1 – 4 July 2019

Institute of Nuclear Physics
Polish Academy of Sciences



Multis 2019



**Institute of Nuclear Physics
Polish Academy of Sciences**



**Multiscale phenomena in molecular matter
Kraków, 1 – 4 July 2019**

Programme and abstract book

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Dear Colleagues, dear Friends,

It is our great pleasure and honour to welcome you to the conference "**Multi-scale phenomena in molecular matter**", held in Kraków 1 – 4 July 2019. We are happy that you found our idea of a scientific meeting devoted to a wide scope of research into molecular materials interesting and worth joining. We are very grateful to those of you who accepted our invitation to present a keynote or invited lecture: it was an important point at the beginning of organization and helped us a lot, thank you. The rich subject area of the conference, comprising structure, dynamics, relaxation, magnetism, acoustics and other properties, as well as great diversity of materials, from liquid crystals to molecular nanomagnets, and a variety of experimental techniques, reflects somehow the investigations we have been conducting in the Institute of Nuclear Physics for a long time. A series of biennial conferences dedicated to studies of molecular dynamics and related problems by neutron scattering and complementary methods was organized and animated by our Professor, late Jerzy Janik. Investigation of condensed and molecular matter is a very active area of research. Thanks to the increasingly advanced experimental and computational techniques it became an interdisciplinary field. Our intention is to promote collaborative research among physicists, chemists and natural scientists, which may bring new ideas and important results.

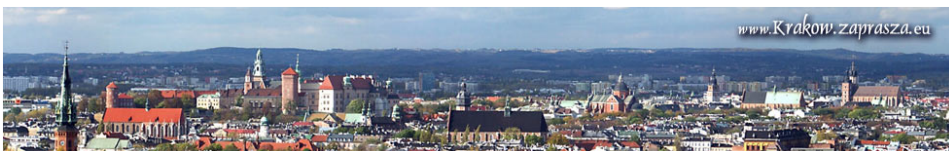
The conference is organized by the Institute of Nuclear Physics, Polish Academy of Sciences. The Institute was established in 1955, the founder and first director was Professor Henryk Niewodniczański. Even though the main research concerns particle and nuclear physics, the condensed matter physics together with other disciplines like nano-materials engineering, dosimetry or medical physics, is being explored as well. On the day of the opening of the conference we will visit the youngest division of the Institute, the Bronowice Cyclotron Centre dedicated to basic research and tumour radiotherapy.

We welcome all of you to the conference and firmly hope that Multis 2019 will be an important and valuable scientific event. We expect that lectures and posters will initiate interesting and stimulating discussions. During the conference you are invited to see the historical places in our beautiful city, therefore we wish you an inspiring and enjoyable time in Kraków.

R. Pietucha

The historical panorama of Kraków at the Welcome page is a copy of the copperplate engraving by Meriam Matthaus Elder. In 1619 he wrote „Cracovia Totius Poloniae urbs celeberrima atque amplissima regia atque Academia insignis” (Most celebrated and splendid city in all Poland notable by the royal castle and Academia).

Design of our Logo was inspired by the mosaic from Pompeii (Casa degli Amorini Dorati) as it mimics the multiscale path. The T_EX code to draw the mosaic was first published by Daniel Steger <http://www.texample.net/tikz/examples/mosaic-from-pompeii>



Sightseeing & Social program

Monday, 1 July 2019, 16:10

After the opening part of the conference including an opening lecture and/or a visit to the Cyclotron Centre Bronowice, you are invited to the Welcome Party. It will take place on the premises of the Institute of Nuclear Physics in front of its main entrance.

Wednesday, 3 July 2019, 15:00

The best part of Wednesday afternoon is devoted to a visit to the Renaissance castle in Pieskowa Skała (Polish for Little Dog's Rock). It is located within the boundaries of the Ojców National Park, 27 km north of Kraków. The castle was first mentioned in Latin documents of Polish king Władysław I the Elbow-high before 1315, as castrum Peskenstein. The castle was built by King Casimir III the Great in the first half of the 14th century. It is part of the chain of fortified castles along the Trail of the Eagle's Nests, along the highland plane of the Polish Jura extending north-west from Kraków to the city of Częstochowa. The castle changed hands many times over the centuries. In 1903 it was bought by the Pieskowa Skała Society led by Adolf Dygasiński and with time it was turned over to the Polish state and meticulously restored. After lunch, at 14:40, we will be driven right to the spot. On arrival at Pieskowa Skała, you will be invited to visit some parts of the castle together with the local museum. Thereafter the conference dinner will be served in the local restaurant.

Thursday, 4 July 2019, 17:00

The Multis 2019 conference closing will be held in the assembly hall of the Institute. During the meeting the prizes for the best posters will be awarded and plans for a follow-up meeting will be announced.



Programme of the Conference

MONDAY, 1 JULY 2019

- 12:00 **Registration:** Institute of Nuclear Physics Polish Academy of Sciences, Entrance Hall
- 15:00 **Opening of the Conference:** Institute of Nuclear Physics Polish Academy of Sciences, Assembly Hall
- 15:10 **Tom Lancaster**, Low dimensional and topological states in molecular magnets p. 18
- 16:10 **Visit to the Cyclotron Centre Bronowice**
- 16:10 **Welcome party:** Institute of Nuclear Physics Polish Academy of Sciences

TUESDAY, 2 JULY 2019

Session: SOFT MATTER & APPLIED PHYSICS

- 09:00 **Marian Paluch**, On decoupling phenomenon between charge transport and structural dynamics in protic ionic liquids p. 20
- 09:40 **Małgorzata Śliwińska-Bartkowiak**, Structures of ice confined in nanopores p. 22
- 10:10 **Wycliffe K. Kipnusu**, Laser fabrication of carbon nanostructures for fluorescence-based tear glucose sensor p. 24
- 10:40 **Hal Suzuki**, Dynamics and thermodynamics of Li^+ and H_2O encapsulated in fullerene C_{60} at low temperature p. 26
- 11:00 **Łukasz Kolek**, Molecular dynamics of the antiferroelectric 2F5 liquid crystal p. 28
- 11:20 Coffee break

Session: NANOMAGNETS, NANOSTRUCTURES & CONDUCTORS

- 11:50 **Eva Pavarini**, Building and solving realistic many-body models for molecular nanomagnets p. 30
- 12:30 **Atsushi Kawamoto**, Site-selective NMR and its application to organic conductors p. 32
- 13:00 **Yasuhiro Nakazawa**, Thermodynamic investigations of the gap-symmetry of molecule-based superconductors p. 34
- 13:20 **Michał Krupiński**, Domain structure and magnetization reversal of Co/Pd antidots with perpendicular magnetic anisotropy p. 36
- 13:40 Lunch break

Session: MULTIFUNCTIONAL MATERIALS & SPECTROSCOPY

- 15:00 **Silvia Borsacchi**, Solid State NMR spectroscopy: a multiscale "lens" for understanding complex materials p. 38

15:30	Aleksandra Pajzderska , Structural and dynamical properties of selected drugs confined in ordered mesoporous silica matrix	p. 40
16:00	Christopher Stanton , Control of the generation and detection of coherent phonons through external magnetic fields	p. 42
16:20	Marco Geppi , Starch/sucrose amorphous blends studied by low- and high-resolution Solid State NMR	p. 44
16:40	Tetiana Nagorna , Clustering processes of fullerenes C ₆₀ and C ₇₀ in toluene/N-methyl-2-pyrrolidone mixture by SANS, SAXS, UV-Vis and DLS data	p. 46
17:00	Technical break	
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17:25	Oleksandr Pastukh , Synthesis in silica nanoreactors: how to fabricate precise multifunctional materials?	p. 52
17:35	Michał Żurek , Automatic apparatus for studying the sorption properties of intermetallic compounds	p. 138
17:50	POSTER SESSION	

WEDNESDAY, 3 JULY 2019

Session: GLASS-FORMERS & SOFT MATTER

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09:40	Thomas Blochowicz , Depolarized dynamic light scattering and dielectric spectroscopy: two perspectives on molecular reorientation in supercooled liquids	p. 58
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11:00	Coffee break	

Session: MULTIFUNCTIONAL MAGNETIC MATERIALS

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12:10	Jaume Veciana , Electronic transport through organic spin-containing molecules and their use for manipulating electronic properties of surfaces	p. 66

12:40	Magdalena Laskowska , Multifunctional nanocomposites based on ordered mesoporous silica — synthesis and characterization	p. 68
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13:20	Marc Morant-Giner , Functionalization of MoS ₂ with molecular-based systems: towards tuneable composites	p. 72
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Session: NEW IDEAS, MAGNETISM

09:00	Shoichi Kutsumizu , Cubic phases formed by chain-core-chain type molecules — formation mechanism and molecular design	p. 74
09:40	Eric Čížmár , Pinned solitons in genuine organic anion-radical salt (Et-2,6-diMe-Pz)(TCNQ) ₂	p. 76
10:10	Munetaka Oyama , Noble metal modified nickel electrodes for electrocatalysis	p. 78
10:40	Andrzej Szytuła , Influence of nano-particle size on the properties of multiferroic TbMnO ₃	p. 80
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12:50	Dominika Kuźma , The switching mechanism of finite and infinite chains of macrospins	p. 86
13:10	Maciej Majka , Spatially correlated stochastic dynamics in self-assembly and glass transition	p. 88
13:40	Lunch break	

Session: NEUTRON SPECTROSCOPY & MOLECULAR MAGNETS

15:00	Tatiana Guidi , Neutron spectroscopy of single and entangled antiferromagnetic rings	p. 90
15:30	Randy Fishman , Magnetic interactions and spin dynamics of the multiferroic (NH ₄) ₂ FeCl ₅ (H ₂ O)	p. 92
16:00	Żaneta Świątkowska-Warkocka , Magnetic properties of hybrid particles prepared by pulsed laser irradiation methods	p. 94
16:20	Closing	

Poster session

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1. **Juliusz Chojenka**, Study of the structure of titanium thin films deposited by e-beam PVD p. 96
2. **Dominik Czernia**, Zero-field magnetic susceptibility of molecular chain magnet Cu(II)-Fe(III) in the semiclassical model of isotropic chains p. 98
3. **Elżbieta Drzymała**, Ternary Pt/Re/SnO₂/C system as an effective catalyst for application in fuel cells p. 100
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7. **Wenbin Guo**, Polymorphism and light-induced spin transition in [Fe(Pm-*p*BrA)₂(NCS)₂]. Towards high T (LIESST) p. 108
8. **Gabriela Handzlik**, Slow magnetic relaxation in a gadolinium(III)-dioxophenanthroline qubit candidate p. 110
9. **Ewa Juszyńska-Gałązka**, Low temperature polymorphism and dynamic of lithocholic acid (LCA) p. 112
10. **Jan Łażewski**, Destructive influence of the edge dislocation on 4H-SiC properties — DFT study p. 114
11. **Yuki Matsumura**, Mott criticality and glassy features of phonons induced by electron correlations in molecule-based superconductors studied by heat capacity measurements p. 116
12. **Mark W. Meisel**, Exploring enhanced magnetocaloric effect in low dimensional magnets as potential refrigerants in high magnetic fields p. 118
13. **Tetsuya Nomoto**, Thermodynamic properties of organic conductors with charge fluctuation p. 120

14. **Paweł Pakulski**, Bis(triphenylphosphine)iminium salts of dioxthiadiazole radical anions p. 122
15. **Marcin Piwowarczyk**, Mesomorphism and photochemistry of (E)-4-((4-octyloxyphenyl)diazenyl)phenyl alkanotes p. 124
16. **Andrzej Ptok**, Formation of the Majorana bound states on defects p. 126
17. **Aleksandra Radko**, Self-assembled patterns of monolayer prepared on solid surface from DNA-CTMA complex p. 128
18. **Wojciech Sas**, Structural and magnetic properties of Prussian blue analogue $\text{Fe}_3[\text{Cr}(\text{CN})_6]_2 \cdot n\text{H}_2\text{O}$ thin films obtained by electrodeposition and ion-exchange synthesis p. 130
19. **Paweł Sobieszczyk**, Magnetization reversal mechanism in nanopatterned multilayer with PMA and different antidots lattice symmetry p. 132
20. **Małgorzata Sternik**, Ab initio and nuclear inelastic scattering studies of $\text{Fe}_3\text{Si}/\text{GaAs}$ heterostructures p. 134
21. **Piotr M. Zieliński**, Thermal instability of carbamazepine p. 136
22. **Michał Żurek**, Automatic apparatus for studying the sorption properties of intermetallic compounds p. 138

Low dimensional and topological states in molecular magnets

T. Lancaster

Durham University, Durham, UK

Low-dimensional quantum magnetism continues to be of great theoretical and experimental interest, as reduced dimensionality supports strong quantum fluctuations that can result in novel excitations and critical behaviour. Of particular recent importance is the understanding the physics in reduced dimensions using notions from topology. Examples include topological objects such as walls, vortices and skyrmions, which exist in the spin textures of a range of magnetic systems, and one-dimensional spin chain systems, where topological considerations are key in elucidating the possible ground states and excitation spectra. Here we discuss our recent results in this area, with an emphasis on the use of muon-spin relaxation as a sensitive probe of emergent magnetism in spin chains and ladders. Muons have repeatedly been shown to be sensitive to long-range magnetic order in these systems, which is often very difficult to observe using other techniques, and also to low-energy dynamics.^(1,2)

We present the results of measurements on a series of gapped molecular materials, including: (i) $\text{Cu}(\text{pyz})(\text{gly})\text{ClO}_4$ which is based on spin dimers;⁽¹⁾ (ii) the spin ladder material $(\text{Hpip})_2\text{CuBr}_4$ ⁽²⁾ where similar physics governs the phase diagram; and (iii) the chiral spin chain $[\text{Cu}(\text{pym})(\text{H}_2\text{O})_4]\text{SiF}_6 \cdot \text{H}_2\text{O}$.⁽³⁾ We use our muon spectra to identify the regions of the phase diagram and crucially, we show that density functional theory can be used to explain how perturbations to a material caused by the presence of the charged muon impurity, allow the muon to probe the system. We also present new results on a $S = 1$ molecule-based magnet which is a successful realization of a Haldane spin chain.⁽⁴⁾ By applying magnetic fields we are able to close the Haldane spin gap, driving the system through a quantum critical point. We discuss the prospects for gaining control over such molecule-based systems via chemical engineering, with an aim to promote exotic ground states.

⁽¹⁾ T. Lancaster et al., Phys. Rev. Lett. 112 (2014), 207201.

⁽²⁾ T. Lancaster et al., New. J. Phys. 20 (2018), 103002.

⁽³⁾ J. Liu et al., Phys. Rev. Lett 122 (2019), 057207.

⁽⁴⁾ R. C. Williams et al., in preparation (2019).

KEYNOTE LECTURE, TUE./09:00

On decoupling phenomenon between charge transport and structural dynamics in protic ionic liquids

M. Paluch

University of Silesia, Katowice, Poland

Protic ionic liquids (PILs) are a special subgroup of ionic liquids. They are formed by transfer of protons from Brønsted acids to Brønsted bases. Since this process is reversible, it can result that PILs consist of not only cations and anions but may also contain neutral, un-ionized molecules. If the amount of neutral molecules is significant it is expected that such liquids should exhibit rather low electrical conductivity and, consequently, they are classified as a "poor" ionic liquids. However, the conductivity of PIL depends not only on the degree of proton transfer from the acid to the base but also on hydrogen bonding in which proton is involved provided that given PIL also forms hydrogen bonds. In the last case, the proton has anomalously high mobility resulting in very high electrical conductivity. This may also lead to the decoupling of electrical conductivity and the structural relaxation. In this talk we present both the conductivity and structural relaxation measurements of a number of PILs performed as a function of temperature and pressure. To investigate charge transport and the structural dynamics we employed Broadband Dielectric Spectroscopy and Dynamic Light Scattering, respectively. As a result we found that the decoupling of electrical conductivity from structural relaxation time becomes more pronounced with increasing pressure.^(1,2) This finding shows that the fractional Debye Stokes Einstein law is violated. Consequently we propose a new approach based on the thermodynamic scaling concept for analysis the correlation between electrical conductivity and structural relaxation time.

⁽¹⁾ Dielectric properties of Ionic Liquids. Ed. Marian Paluch, Springer-Verlag, 2016.

⁽²⁾ Z. Wojnarowska, M. Rams-Baron, J. Knapik-Kowalczyk, A. Połatyńska, M. Pochylski, J. Gapiński, A. Patkowski, P. Włodarczyk, M. Paluch, Scientific Reports 7 (2017), 7084.

Structures of ice confined in nanopores

M. Śliwińska-Bartkowiak,¹ K. Domin,¹ M. Jazdzewska,¹
A. Beskrovnyi,² K. E. Gubbins³

¹Faculty of Physics, Adam Mickiewicz University, Poznań, Poland

²Joint Institute for Nuclear Research, Dubna, Russia

³Department of Chemical & Biomolecular Engineering, North Carolina State University, Raleigh, USA

We report X-rays diffraction studies of water adsorbed in nanoporous activated carbon fibres (ACFs) and CMK-3 and CMK-8 carbon mesopores of different pore sizes. The fibres are built of turbostratic nanoparticles separated by quasi two-dimensional voids, forming narrow slit-shaped pores; CMK-3 and CMK-8 are the reverse carbon replica of silica SBA-15 and KIT-6 porous matrices. In order to determine the structure of water within the pores and its influence on the fibres' structure, mean interatomic and intermolecular distances have been estimated from the positions of the maxima of the normalized angular distribution functions obtained by X-ray diffraction.⁽¹⁾ We observe significant changes in the interlayer distance of the carbon nanoparticles; the results suggest that very high pressures arise within the pores, of the order a few hundreds MPa, as has been observed in molecular simulations.^(1,2) Such results are confirmed by observation of high pressure forms of ice in cylindrical nanocarbons, using neutron and X-ray diffraction. For water in multi-walled carbon nanotubes (MWCN), below the pore melting point cubic ice was observed. This structure of ice can be obtained during re-crystallisation from high pressure phases at low temperature for bulk water. For CMK-3 and CMK-8 mesopores we observed the existence of a stacking-disordered ice, I_{sd} .^(3,4) This metastable ice is neither cubic nor hexagonal, and is not a simple mixture of the two, but a combination of cubic sequences intertwined with hexagonal sequences, which was identified as having the space group $P3m1$.⁽³⁾ Moreover, the stacking disorder can vary in complexity depending on the way the ice is formed and on the prevailing thermal conditions during this process. An analysis of the kind of I_{sd} formed in CMK-3 and CMK-8 of different pore sizes and also in ACF will be presented. These crystal forms, which occur in bulk water only at temperatures below 180 K in the case of cubic ice, and at pressures of hundreds or thousands of MPa are stabilized by the confinement.

Financial support from the National Centre of Science, grant No. UMO-2016/22/A/ST4/00092 is gratefully acknowledged.

- (1) M. Sliwinska-Bartkowiak, M. Drozdowski, M. Jazdzewska, Y. Long, J. Palmer, K. E. Gubbins, *Phys. Chem. Chem. Phys.* 14 (2013), 71454.
- (2) Y. Long, J. Palmer, B. Coasne, M. Sliwinska-Bartkowiak, K. E. Gubbins, *Phys. Chem. Chem. Phys.* 14 (2011), 17163; M. Jazdzewska, M. Sliwinska-Bartkowiak, A. Beskrovny, S. G. Vasilovskiy, S. W. Ting, K. Y. Chan, L. L. Huang, K. E. Gubbins, *Phys. Chem. Chem. Phys.* 13 (2011), 9008.
- (3) T. L. Malkin, B. J. Murray, C. Salzmann, V. Molinero, S. J. Pickering, T. F. Whale, *Phys. Chem. Chem. Phys.* 17 (2014), 60; A. Haji-Akbari, P. G. Debenedetti, *PNAS*, 112 (2015), 10582.
- (4) K. Domin, K. Y. Chan, H. Yung, A. Sterczynska, M. Jurek, K. E. Gubbins, M. Sliwinska-Bartkowiak, *J. Chem. Eng. Data*, 61 (2016), 4252; M. Jazdzewska, K. Domin, M. Sliwinska-Bartkowiak, A. Beskrovny, *J. Mol. Liquids* (2018), in press.

INVITED LECTURE, TUE./10:10

Laser fabrication of carbon nanostructures for fluorescence-based tear glucose sensor

W. K. Kipnusu

Universität Jaume I, Valencia, Spain

Highly fluorescent nanocomposite consisting of carbon nanostructures are fabricated by simultaneous pulsed laser ablation in liquids and disruptive femtosecond technology. This is an environmentally green method that promotes "green" technologies for nanoparticles synthesis. The prepared nanocomposite are applied for noninvasive glucose sensing for diagnosis and management of diabetes. The prevalence of diabetes is continuously rising even in low-income economies therefore the blood glucose monitoring tools are in high social demand globally. Uninterrupted monitoring of blood glucose is a must in order to keep the fatal levels of glycated hemoglobin under control and improve the quality of life for diabetic patients. However, this monitoring is compromised by the painful finger pricking about 4 – 5 times a day to obtain blood samples which leads to patient non-compliance and hence endangering their lives. A discussion of a relatively pain-free non-invasive blood glucose monitoring through in vitro sensing of tear glucose by fluorescence technique will be discussed.

INVITED TALK, TUE./10:40

Dynamics and thermodynamics of Li^+ and H_2O encapsulated in fullerene C_{60} at low temperature

H. Suzuki

Department of Chemistry, Kindai University, Osaka, Japan

email: h_suzuki@chem.kindai.ac.jp

Atoms or molecules encapsulated in a nanospace exhibit distinctly different properties from those in the bulk state. If the space inside a cage is large enough compared to the size of an encapsulated (guest) molecule, the guest molecule can move around in the cage even at low temperature, exhibiting quantized motions. When the cage (host) molecules are condensed to form a crystalline phase, weak interactions between the guest molecules may have a chance to contribute to those quantum motions. From a thermodynamic point of view, free motions inside a cage is entropically preferred, while the localization due to the guest-guest or guest-host interaction is energetically preferred. This thermodynamic balance varies with temperature, which can induce an order-disorder phase transition. Such transitions are expected to be influenced not only by the type of guest molecules, but also by the size and symmetry of the space inside host cages as well as their distances. Fullerene C_{60} is one the ideal cages to examine these contributions, because its inner space is approximately spherical and various co-crystal structures can be formed by adding small spherical molecules.

Recently we have investigated the dynamics and thermodynamics of a Li^+ ion and a H_2O molecule encapsulated in a fullerene C_{60} by spectroscopic and calorimetric measurements.^(1,2) In $[\text{Li}^+\text{@C}_{60}](\text{PF}_6^-)$ crystal, Li^+ ions was found to rotate in the C_{60} cage above 150 K, while it localizes into two sites below 100 K and into one site below 24 K exhibiting antiferroelectric ordering. In $\text{H}_2\text{O@C}_{60}$ crystal, on the other hand, H_2O molecule was found to exhibit quantum rotation even at 2 K. It also shows nuclear spin interconversion between ortho and para states below 20 K.

⁽¹⁾ H. Suzuki, M. Ishida, M. Yamashita, C. Otani, K. Kawachi, Y. Kasama, E. Kwon, PCCP 18 (2016), 31384.

⁽²⁾ H. Suzuki, M. Nakano, Y. Hashikawa, Y. Murata, J. Phys. Chem. Lett. 10 (2019), 1306.

CONTRIBUTED TALK, TUE./11:00

Molecular dynamics of the antiferroelectric 2F5 liquid crystal

Ł. Kolek,¹ K. Dychtoń,¹ M. Jasiurkowska-Delaporte,² W. Szaj,¹
A. Bąk¹

¹Rzeszów University of Technology, Poland

²Institute of Nuclear Physics Polish Academy of Sciences, Kraków,
Poland

The complex molecular dynamics of (2S)-octano-2-yl4'-(2-fluoro-4-{ [5-(1,1,2,2,3,3,3 heptafluoropropoxy)pentyl]oxy }benzoyloxy)-[1,1'-biphenyl]-4-carboxylate, abbreviated as 2F5, has been studied by broadband dielectric spectroscopy (BDS). 2F5 shows rich polymorphism of liquid-crystalline and glassy phases. Studies by DSC and polarizing microscopy methods revealed the following phase sequence on cooling: SmA*, ferroelectric SmC*, antiferroelectric SmC_A* and the glassy GSmC_A* phases. During heating of the sample two scenarios are observed: on slow heating rates ($\phi < 1.5$ K/min) the cold crystallization of crystal Cr from metastable SmC_A* phase and then the transition to stable SmC_A* occur while in the case of higher heating rates, SmC_A* does not crystallize and it transforms directly to the ferroelectric SmC* phase. In frequency range from 10^{-1} to $3 \cdot 10^6$ Hz two relaxation processes were detected in liquid-crystalline smectic phases. The processes observed in SmA* and SmC* phases were identified as a soft mode and Goldstone mode, respectively. Three AFM relaxation processes were detected in the antiferroelectric SmC_A* phase. The slowest of them has Arrhenius-like behavior, while two faster processes show a super-Arrhenius character. In the glass state of the SmC_A* phase, the secondary β -relaxation process was detected. The dielectric glass transition temperature values determined from the VFT equation for AFM2 and AFM3 relaxation processes coincide with the T_g value obtained from the DSC method.

Acknowledgements: Ł. K. and M. J-D acknowledge the National Science Centre (Grant SONATA11: UMO-2016/21/D/ST3/01299) for financial support.

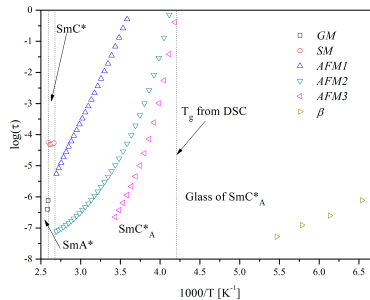


Figure 1. Arrhenius plot for processes observed during slow cooling in the liquid-crystalline and glassy phases.

KEYNOTE LECTURE, TUE./11:50

Building and solving realistic many-body models for molecular nanomagnets

E. Pavarini

Institute for Advanced Simulation and JARA High-Performance Computing, Germany

Strongly-correlated molecular nanomagnets are ideal test beds to investigate fundamental issues in quantum mechanics. During the last years sophisticated experiments and targeted research activities have unveiled a variety of fundamental quantum phenomena and potential technological applications of these materials. Furthermore, impressive advances in the field of molecular spintronics allow us to study electron transport through individual magnetic molecules embedded between metallic leads, even in the purely quantum regime of single electron tunneling. The theoretical description of these systems in a truly realistic setting remains, however, a challenge.

In this talk, I will present a flexible and effective scheme to build ab-initio many-body models for these systems — and obtain the corresponding low-energy magnetic Hamiltonians. It is based on using localized Foster-Boys orbitals as a one-electron basis.⁽¹⁾ I will illustrate applications of the method to some paradigmatic systems, such as the antiferromagnetic rings $\{\text{Cr}_8\}$ and $\{\text{Cr}_7\text{Ni}\}$, the single-molecule magnet $\{\text{Fe}_4\}$, and two $\{\text{Cr}_7\text{Ni}\}$ -Ni- $\{\text{Cr}_7\text{Ni}\}$ assemblies.⁽¹⁻⁴⁾ Finally, I will present recent extensions of the technique to the calculation of electron transport in the single electron tunneling regime.⁽⁵⁾

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INVITED LECTURE, TUE./12:30

Site-selective NMR and its application to organic conductors

A. Kawamoto

Hokkaido University, Japan

Functional molecular compound are promising materials for not only pure science but also industries and provide many key materials with novel physical properties. Hence the field of functional molecules is a prominent part of condensed matter physics.

Especially, the development of organic conductors realized the superconductivity and provided the samples of the strong correlated electron system, etc.⁽¹⁾ The magnetism gives us important information of the electron spin. Moreover, microscopic experiments are essential for the investigation of the novel physical phenomenon and the elucidation of the mechanism.

Nuclear magnetic moment is one of the best microscopic magnetic probes. For example, Nuclear Magnetic Resonance (NMR) provided the crucial experimental evidence for BCS mechanism⁽²⁾ and ⁵⁷Fe Mössbauer spectrum detects clear internal fields on Fe nuclei with high sensibility.⁽³⁾ Indeed, these experiments are powerful in condensed matter physics and are also effective in the research of the functional molecular materials. Unfortunately, major ¹²C atoms in organic molecules does not have nuclear magnetic moment and NMR active ¹H atoms are not suitable to deflect electron spins due to the small coupling constant. There are many inequivalent C sites in materials. Even if we could get the signal from C, many inequivalent sites make spectrum complicated. It turns, however, the potential disaster to one's advantage. The major NMR inactive ¹²C atoms enable us to do site-selectively substitution with NMR active ¹³C and site-selective NMR. Choosing the substitutional site, we can do the experiments strategically.⁽⁴⁾

As mentioned above, molecular materials with novel physical properties have been developed. We have been developing the site-selective NMR with chemical synthesis and investigated the novel physical properties, providing crucial experimental results.

I would like to introduce our site-selective NMR works on unconventional organic conductors, charge ordered compound and *p-d* systems, and how does it work.

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CONTRIBUTED TALK, TUE./13:00

Thermodynamic investigations of the gap-symmetry of molecule-based superconductors

Y. Nakazawa, T. Nomoto, Y. Matsumura, S. Fukuchi, S. Yamashita, H. Akutsu

Department of Chemistry & Research Center for Thermal and Entropic Science, Osaka University, Japan

We carried out systematic heat capacity measurements of molecule-based charge transfer complexes with D_2X composition, where D and X denote organic donor molecules and monovalent counter anions, respectively. Especially, we focus on the complexes with the κ , β , λ , and θ type arrangements of BEDT-TTF (bis(ethylenedithio)tetrathiafulvalene) and BETS (bis(ethylenedithio)tetraselenafulvalene) donor molecules. The quasi-two-dimensional conductivity and the magnetic features reflecting the difference of the donor arrangements appear in them in various manners. In the case of κ -type and λ -type structure, the organic molecules form a rigidly dimerized structure and electron correlations play important roles to produce superconductivity. On the other side, those possessing non-dimeric structure like θ -type give anomalous metallic features accompanied by large charge fluctuations.

In order to attain accurate heat capacity measurements for single crystalline samples of these charge transfer salts, we constructed a relaxation calorimetry system by fabricating small chip-type resistances. The reduction of the background made it possible to measure the heat capacity of 50 – 300 μg single crystals under magnetic fields. The systematic change of thermodynamic characters of them is discussed in terms of competitive feature of band-picture and Mott-Hubbard picture. We also developed a system to measure angle resolved heat capacity (ARHC) measurements with in-plane magnetic field to determine node and anti-node direction of the superconductive gap. The ARHC detected distinct four-fold periodicity together with the two-fold one which indicate the d -type pairing or $s+d_{x^2-y^2}$ -type pairing in the dimer-based superconductors.

CONTRIBUTED TALK, TUE./13:20

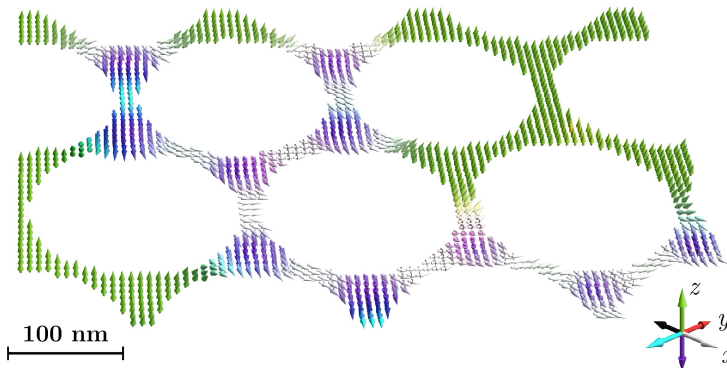
Domain structure and magnetization reversal of Co/Pd antidots with perpendicular magnetic anisotropy

M. Krupiński, P. Sobieszczyk, P. Zieliński, M. Marszałek

Institute of Nuclear Physics Polish Academy of Sciences, Kraków,
Poland

email: Michal.Krupinski@ifj.edu.pl

A micromagnetic model is constructed for antidot arrays with perpendicular magnetic anisotropy, which accounts for intrinsic and extrinsic defects associated with the polycrystalline character of the material including defected edges of nanostructures. The predictions of the model were compared with the measurements obtained for Co/Pd multilayers patterned by nanosphere lithography supported by RF-plasma etching, which provide highly ordered arrays of circular antidots with period of 202 nm. After a careful selection of phenomenological parameters the model accurately reproduces the hysteresis loops and domain pattern in the pristine material, and predicts magnetic parameters and reversal mechanism for hexagonally ordered arrays of antidots. Different micromagnetic modeling approaches showed that magnetic properties and domain configuration in nanopatterned systems with perpendicular anisotropy are strongly determined by defects, heterogeneity of nanostructure sizes, and edge corrugations, and that such imperfections play a key role in processes of magnetic reversal. The domain pattern simulations shed light on the details of magnetic reversal. In particular, an increase in the Néel domain walls, as compared to Bloch walls, was observed with a decrease of the distances between the antidots. The simulations indicated that a neck between two antidots can behave like a short nanowire with a width determined by the array period and antidot diameter. The evolution of the domain structures with the intensity of the external field was also visualized, and it was predicted that the antidot lattice geometry connected with defected edges would lead to the formation of structures, such as a network of magnetic bubbles (shown below), which are unstable in non-patterned flat films.



INVITED LECTURE, TUE./15:00

Solid State NMR spectroscopy: a multiscale "lens" for understanding complex materials

S. Borsacchi,¹ F. Martini,² E. Carignani,² L. Calucci,¹ M. Geppi²

¹Italian National Research Council, Institute for the Chemistry of OrganoMetallic Compounds (ICCOM-CNR), Pisa, Italy

²University of Pisa, Department of Chemistry and Industrial Chemistry, Italy

Complexity is a common feature intrinsic to many materials playing a key role in in biology, chemistry and industry. Complexity can arise from many factors as the coexistence of different chemical components and phases and an overall structural disorder and heterogeneity. Because of complexity it is often difficult to obtain a detailed characterization of interesting materials, while, on the other hand, such a knowledge is crucial for understanding the functional performances of materials and orienting their design, synthesis and optimization. Solid State NMR spectroscopy is an extremely powerful technique, which can effectively bridge this gap. Indeed, it can be applied to substantially every kind of material and, by exploiting a plethora of nuclear probes and properties, it allows structural and dynamic properties to be characterized on very wide spatial (0.1 – 100 nm) and frequency (Hz – GHz) scales.^(1–4) In this contribution I will try to highlight the power and significance of this technique, going through several studies, carried out in our research group, in which Solid State NMR has allowed a multiscale understanding of innovative complex materials.^(5–7)

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INVITED LECTURE, TUE./15:30

Structural and dynamical properties of selected drugs confined in ordered mesoporous silica matrix

A. Pajzderska

Faculty of Physics, A. Mickiewicz University, Poznań, Poland

Ordered mesoporous silica materials are an important type of functional materials with a regular porous structure characterized by a uniform pore size ranging from 2 to 50 nm, along with a large surface area and good physicochemical stability. They are used in many fields including biotechnology, material engineering, photonics or nanomedicine, as well as the systems for storing and converting energy or environment remediation. Due to their considerable biocompatibility and biodegradability they can also be used as drug delivery systems. One of the major advantages of encapsulating the drug substance in silica matrices is potentially the increasing of solubility and bioavailability — important parameters for the pharmaceutical industry.

Structural and dynamical properties of selected crystalline and drugs confined in SBA-15 matrix (e.g. nimodipine, ranitidine hydrochloride, carbimazole) were studied by different experimental and computational techniques, in particular, systems were characterized by calorimetry, powder X-ray diffraction, ^{13}C and ^1H solid-state NMR, quasielastic neutron scattering spectroscopy (QENS) and molecular simulations methods (MD). The combining ^1H NMR relaxometry and QENS with theoretical modeling allowed a quantitative description of experimental data.

In the crystal sample, the molecular dynamics can be mainly attributed to the reorientation of the methyl groups. For confined drugs the reduction of intermolecular interactions and the loss of the crystal packing were observed. It leads to the reduction of the activation energies for the methyl groups. Due to conformational changes and getting additional degrees of rotational freedom with respect to the bulk one, the reorientation of the molecular fragments and/or the entire molecules were also detected.^(1–6)

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INVITED TALK, TUE./16:00

Control of the generation and detection of coherent phonons through external magnetic fields

C. Stanton

Department of Physics, University of Florida, USA

email: stanton@phys.ufl.edu

Ultrafast, femtosecond laser spectroscopy is a powerful tool for studying the dynamics and fundamental interactions of carriers, spins and phonons in a wide variety of materials. The decay of the transmission or reflection of a probe pulse as a function of probe delay time can provide important insight into the carrier/spin relaxation processes. Often times, superimposed on the decay signal of the probe pulse is a signal that oscillates in time. These oscillations are known as *coherent phonons* and can be used to probe and provide information on the quality of *surfaces and interfaces* and internal fields far below the surface. The ability to control these coherent phonons and hence the vibrational, thermal and phononic properties of materials has potentially important technological impacts. Possible applications include heat management; charge transfer; and phonon-lasing. Methods of tailoring and controlling vibrational properties in the past have relied on inter-digitated transducers to generate surface acoustic waves in a variety of applications. We experimentally and theoretically studied the generation and control of longitudinal coherent acoustic phonons generated by ultrafast laser using external magnetic fields. The sample studied was a semiconductor heterostructure, consisting of a heavily p-doped ferromagnetic GaMnAs layer grown on an intrinsic GaAs substrate. Using two-color Time Resolved Differential Reflectivity (TRDR) measurements we observed oscillations whose magnitude, frequency, and phase were functions of the applied magnetic field. Theoretical modeling was based on an 8 band $\mathbf{k} \cdot \mathbf{P}$ calculation for the electronic structure including external magnetic field and the $sp - d$ exchange interaction between the electron/hole spin with Mn spin. The carrier phonon propagation and dynamics and its effect on the reflectivity was also modeled. Comparison of calculations to experiment demonstrate that the phase, frequency and amplitude of the CP oscillations can be controlled with external magnetic fields and Mn doping.

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Work done in conjunction with H. Petek (U. Pittsburgh), K. Ishioka (NIMS), B. A. Magill (Virginia Tech.) G. A. Khodaparast (Virginia Tech.), S. Thapa (U. Florida).

CONTRIBUTED TALK, TUE./16:20

Starch/sucrose amorphous blends studied by low- and high-resolution Solid State NMR

M. Geppi,¹ F. Martini,¹ G. Badolato-Bönisch,² D. J. Hughes,³
J. Ubbink⁴

¹Dipartimento di Chimica e Chimica Industriale, Università di Pisa, Italy

²DSM Nutritional Products, Kaiseraugst, Switzerland

³H. H. Wills Physics Laboratory, University of Bristol, UK

⁴Food Science and Nutrition Department, California Polytechnic State University, USA

email: marco.geppi@unipi.it

Biopolymer-based systems are today encountered in a wide variety of possible applications, since they are usually low-cost materials and respond to the actual eco-sustainable requirements of renewability and biodegradability. In particular, glassy matrices for the encapsulation and stabilization of bioactive compounds often consist of molecularly miscible blends of a carbohydrate of higher molecular weight and a low molecular weight carbohydrate or polyol. The optimization of the barrier properties of such matrices depends in a subtle way on the balance between the plasticization and antiplasticization of the high molecular weight carbohydrate by the low molecular weight compound.⁽¹⁾ To this aim, understanding the phase properties, as well as the structural and dynamic features of these systems at a nanometric and sub-nanometric level is crucial to predict their final macroscopic behaviour.

In this work,^(2,3) the phase, dynamic and miscibility properties of modified food starch/sucrose spray dried amorphous blends were investigated by means of solid-state NMR (SSNMR) techniques. In particular, ¹H and ¹³C high- and low-resolution SSNMR experiments, carried out at different temperatures on blends with different modified food starch/sucrose ratios, gave interesting information on the properties of the starch and sucrose domains and on the degree of interaction between the two components. ¹³C MAS spectra gave information about the amorphicity of the phases and the inter-molecular interactions. ¹H FID's, recorded under on-resonance conditions, showed evidences of the presence of domains with different degree of mobility, whose properties and relative content depend on composition. In addition, the measurement of ¹H T_1 revealed information on the phase separation of the system on the nanometric scale and on the changes induced by molecular interactions on the MHz dynamic behaviour.

The NMR results were supported by and compared with those obtained by other techniques, and in particular by Differential Scanning Calorimetry⁽⁴⁾ and Positron Annihilation Lifetime Spectroscopy.⁽⁵⁾

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CONTRIBUTED TALK, TUE./16:40

Clustering processes of fullerenes C_{60} and C_{70} in toluene/N-methyl-2-pyrrolidone mixture by SANS, SAXS, UV-Vis and DLS data

T. Nagorna,¹ D. Chudoba,¹ O. Kyzyma,¹ L. Bulavin²

¹Joint Institute for Nuclear Research, Dubna, Russia

²Taras Shevchenko National University of Kyiv, Ukraine

Fullerene is a molecular compound consisting of carbon atoms. Along with other allotropic forms of carbon, such as diamond or graphite, fullerenes are the first form, soluble in a wide variety of organic and inorganic solvents. Fullerenes are widely used in various fields, including optics, electronics and medicine.⁽¹⁻³⁾ For these purposes, the production of liquid solutions of fullerenes is necessary.⁽⁴⁾ Despite of a wide application of fullerene solutions, the processes of their aggregation in solvents and the processes of interaction between fullerenes and solvents are still unclear.⁽⁵⁾

In the present work the structure of fullerenes C_{60} and C_{70} in polar and non-polar solvent mixtures was investigated. Toluene and N-methyl-2-pyrrolidone were chosen as solvents. To carry out these tasks the methods of small-angle neutron scattering, small-angle X-ray scattering, dynamic light scattering, and UV-vis spectroscopy were used.

As a result, the correlation was observed between the fullerene aggregates formation and a volume fraction of the nonpolar solvent toluene. The dependence of the structural state of fullerene C_{70} on the polarity of the liquid medium was studied; an increase in the volume fraction of the polar solvent toluene above the threshold value of 70% led to the destruction of the existing large aggregates and the reorganization of the clusters. The obtained data were analyzed in comparison with the previous results for the similar colloidal systems with fullerene C_{60} .

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Temperature-modulated vibrational dynamics of carbamazepine

A. Dołęga, E. Juszyńska-Gałązka, P. M. Zielński

Institute of Nuclear Physics Polish Academy of Sciences, Kraków,
Poland

Carbamazepine — CBZ — is an Active Pharmaceutical Ingredient (API) exhibiting anticonvulsant properties and a model drug concerning studies of pharmaceuticals' polymorphism. There are four well-known polymorphic forms of CBZ,⁽¹⁾ which differ in crystallographic arrangement as well as in physical and biological properties. Unfortunately, all polymorphs of CBZ exhibit low solubility and consequently limited bioavailability. Due to that, studies aiming at solubility enhancement of CBZ are nowadays very popular.^(2,3)

Amorphisation of drug's structure during rapid cooling from melt seems to be one of the easiest ways to obtain better soluble form of the substance. Pharmaceuticals are usually good glass formers and vitrify when cooling at 5, 10 or 20°C min⁻¹. According to our studies,⁽⁴⁾ CBZ totally vitrifies when cooling at the rate 10°C min⁻¹ or higher. Cooling at the rate 5°C min⁻¹ leads to partial crystallization, but the remaining material vitrifies. Unfortunately, CBZ starts to decompose below melting point and due to that it is impossible to obtain pure glass of CBZ from unmodified substance provided by supplier. Interestingly, our work (4) was, to the best of our knowledge, the first one signaling instability problem of CBZ below melting point. All our conclusions were drawn based on DSC, TGA and HS-POM (Hot-stage Polarized Optical Microscopy) measurements. However, to better explain observed phenomena and to determine the products of degradation of CBZ some further studies were necessary.

Temperature-modulated Fourier-Transform Infrared Spectroscopy (FTIR) was employed to investigate vibrational dynamics of carbamazepine. Measurements were conducted in two sequences, with newly prepared sample for every sequence: a) heating-cooling-heating cycle (5°C → 210°C → 5°C → 210°C); and b) heating — isothermal cycle (5°C → 210°C → isothermal event for 2 hours at 210°C). First cycle aimed at exploring phase sequence, whereas the second one gave an insight into probable products of degradation of CBZ.

Analysis of FTIR measurements was conducted in few different ways: a) changes of positions of C=O stretching bond (≈ 1690 cm⁻¹) and -NH₂ bending bond (≈ 1590 cm⁻¹) during temperature modulation reflected the changes in the strength and amount of intermolecular hydrogen bondings, b) deconvolution of 700 – 820 cm⁻¹ frequency region as well as two dimensional moving window analysis (2DMW) led to determination of phase sequence, c) two dimensional correlation analysis (2DCA) enabled determination of those vibrations which intensities change the most during phase transitions as well as the order of signal alteration.

Shortly, results of FTIR measurements were in good agreement with results obtained using DSC.⁽⁴⁾ Especially, decomposition of CBZ at the temperature lower than previously assumed in the literature was confirmed. Isothermal event at 210°C

showed, that CBZ decomposes at that temperature to iminostilbene. The second product of degradations is probably isocyanic acid which evaporates rapidly and does not contribute to observed FTIR spectra.

Acknowledgments: AD has been partly supported by the EU Project POWR.03.02.00-00-I004/16

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CONFERENCE COMMUNICATION, TUE./17:15

Polymorphism and light-induced spin transition in $[\text{Fe}(\text{Pm-}p\text{BrA})_2(\text{NCS})_2]$. Towards high $T(\text{LIESST})$

W. Guo,¹ N. Daro,¹ S. Pillet,² K. Chainok,¹ M. Marchivie,¹
G. Chastanet,¹ P. Guionneau¹

¹CNRS, Univ. Bordeaux, ICMCB, France

²Université de Lorraine, CNRS, CRM2, Nancy, France

email: wenbin.guo@icmcb.cnrs.fr

The Spin Cross Over (SCO) phenomenon is a change of the electronic configuration of a metal ion from the high-spin state (HS) to the low-spin state (LS) that can be induced by external stimulation, including thermal, light and pressure. Among them, light-induced excited spin-state trapping (LIESST) is usually observed only at low temperature. It is a great challenge to enhance the temperature of LIESST ($T(\text{LIESST})$) towards higher temperature. $T(\text{LIESST})$ is greatly determined by the nature and the geometry of the inner coordination sphere, which can be strongly perturbed by structural motions and intermolecular interactions.^(1,2)

Two new polymorphs of mononuclear compound $[\text{Fe}(\text{Pm-}p\text{BrA})_2(\text{NCS})_2]$ were designed and crystallized with $\text{Pm-}p\text{BrA}=(4\text{-Bromophenyl})\text{-pyridine-2-ylmethylene-amine}$. Polymorphs A and B crystallizes in monoclinic space group with two independent crystallographic sites for Fe(II) in the asymmetric unit. A shows an abrupt hysteretic spin transition around 175 K and a high $T(\text{LIESST})$ at 110 K, probably one of the highest $T(\text{LIESST})$ in family of bidentate ligand. The crystal structure was investigated in the HS and LS states and also in the quenched HS* state showing that the spin-transition is associated to a reversible and large rotation of one part of the ligand. It also appears that the Fe(II) site shows a high distortion of the coordination sphere that could be related to the unusually high $T(\text{LIESST})$. On the contrary, polymorph B shows a gradual SCO without LIESST effect. The comparison of the variable temperature crystallographic investigations indicates clearly differences between the structural properties of A and B notably showing that the different magnetic behaviors originate from the ligand conformation modification during SCO. Furthermore, the close examination of the structure-properties relationships in A and B gives crucial indications for the design of high $T(\text{LIESST})$.

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Synthesis in silica nanoreactors: how to fabricate precise multifunctional materials?

O. Pastukh,¹ M. Laskowska,¹ S. Turchuk, Ł. Laskowski¹

¹Institute of Nuclear Physics Polish Academy of Sciences, Kraków, Poland

In the present work, we have shown the synthesis procedure of the geometrically confined nanocrystals. We were able to achieve small nanocrystals (diameter below 5 nm) with desired properties: nickel pyrophosphate shown a strong non-linear optical response⁽¹⁾ and magneto-electric effect⁽²⁾ in the same time, magnetite particles behave as a ferrimagnet (room temperature) despite that their dimension was below 5 nm. It was possible by applying SBA-15 silica as nanoreactors⁽³⁾ allowing for dosing of reagents with atomic precision and applying spatial confinements.

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Automatic apparatus for studying the sorption properties of intermetallic compounds

M. Żurek,¹ A. Budziak,¹ A. Dębski²

¹Institute of Nuclear Physics Polish Academy of Sciences, Kraków, Poland

²Institute of Metallurgy and Materials Science Polish Academy of Sciences, Kraków, Poland

Hydrogen is one of the most promising, future energy carriers. When hydrogen is burned directly, nitrogen oxides and water vapor are produced, while when hydrogen is oxidised in the fuel cells, the by-product is only water vapor. The energy produced from hydrogen belongs to one of the purest methods of energy production and at the same time is inexhaustible. Hydrogen can be produced from fossil fuels (natural gas, oil and coal) as well as in the electrolysis of water. The method of obtaining hydrogen in fermentation processes with the participation of appropriate bacterial strains is also very promising.⁽¹⁾ The nutrient medium for bacteria may be organic waste from the sugar industry or municipal waste. Although the latter method is very pro-ecological, it has its disadvantage. The fermentation products, in addition to hydrogen, are also CO₂/CO or hydrogen sulphide. This is a major obstacle to the efficient storage of hydrogen in metallic compounds. Contaminants can be removed to a large extent, but in some cases even traces of them can be important. Modification of compounds like LaNi₅ toward ternary compositions change alloy hydrogen storage properties and influence resistance to hydrogen contamination.⁽²⁾ In order to investigate the effect of contaminated hydrogen on the sorption storage of AB₅ type metallic compounds (mainly based on LaNi₅), an automatic sorption apparatus was constructed whose operation is based on the Sieverts volumetric method. The schematic diagram of the apparatus, the actual appearance and the first sorption results for compounds LaNi_{5-x}M_x (M: metal) treated with H₂ and CO₂ (with different concentrations) will be presented. In addition, structural and thermodynamic results (*cpT*) will be presented.

Acknowledgement: This work was financed in the frame of the project BIOS-TRATEG2/297310/13/NCBR/2016

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KEYNOTE LECTURE, WED./09:00

Relaxational dynamics in glass-formers on different time and length scales: relation to fragility

V. Novikov

Institute of Automation and Electrometry, Russian Academy of Sciences, Russia

Spatial scale of molecules in glass-formers may significantly influence the steepness of the temperature dependence of the structural relaxation time (fragility). The relationship between polymer dynamics on various length and time scales remains far from clear. The rigid polymer chains are non-ergodic on time scale of segmental relaxation. We show that this leads to unusually high segmental fragility. It falls out of some typical correlations found in low-molecular weight systems. However, fragility of the viscosity that is determined by chain relaxation follows these correlations for chains of any molecular weight. These results suggest that the molecular level relaxation still follows the behavior usual for small molecules even in polymers. The proposed scenario provides a new insight into the specifics of polymer dynamics: the role of ergodicity on different time and length scales.^(1,2) We also compared the intermediate range order scale L found from the static structure factor and the radius of collective structural relaxation at different temperatures in supercooled liquids state of various glass-forming materials.^(3,4) We found that temperature variations in $L(T)$ differ significantly between different glass-forming liquids. However, there is a correlation between relative changes in $L(T)$ and fragility, that suggests a strong connection between temperature variations in static structural correlations and the dynamics of glass-forming liquids. Furthermore, this temperature evolution of the structural correlation length L is consistent with the changes in the size of cooperatively rearranging regions estimated following Adam-Gibbs theory.

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INVITED LECTURE, WED./09:40

Depolarized dynamic light scattering and dielectric spectroscopy: two perspectives on molecular reorientation in supercooled liquids

T. Blochowicz, J. Gabriel, F. Pabst, T. Boehmer, A. Helbling,
P. Zourchang

Technical University Darmstadt, Germany

Broadband Dielectric Spectroscopy (BDS) can be considered the standard and most widespread method to experimentally access molecular reorientation in supercooled liquids and other complex materials as it covers the full dynamic range of time constants from sub picoseconds in a highly fluid liquid to several thousand seconds close to and below the glass transition temperature. Besides BDS, Depolarized Dynamic Light Scattering (DDLS) is able to probe molecular reorientation in a similar dynamic range but instead of probing permanent molecular dipole moments it is sensitive to the molecular optical anisotropy. Due to this fact a comparison of experimental data from both methods yields additional information, revealing details of the dynamics and on the motional mechanism behind certain relaxation processes. Moreover, both methods are sensitive to intermolecular crosscorrelations in very different ways. Therefore, in a combination of both methods it becomes possible to distinguish between generic features of the glass-transition process on the one hand and crosscorrelation effects that are due to particular intermolecular interactions on the other.

This is exemplified for two cases: First, in monohydroxy alcohols, where hydrogen bonding leads to the formation of transient supramolecular structures, only a combination of BDS and DDLS allows to clearly distinguish between the glass-process and the relaxation of suprastructures. Similarly, in systems with large electric dipole moment dynamic crosscorrelations become important in the dielectric spectra and again only a comparison of both methods reveals the underlying generic alpha relaxation, which turns out to show a high degree of universality between many different systems, including hydrogen bonding and van der Waals glass formers.

A further example is given for the case of supercooled ionic liquids, i.e. molten salts, which are liquid at room temperature and are promising for many applications. Again, only a combination of both methods allows to unambiguously disentangle the contribution of molecular reorientation from other polarization features that often mask reorientation in the dielectric spectra, and allows to identify the dynamic signature of self-assembling supramolecular structures, which are discussed in various ionic liquids and are thought to influence the ionic transport properties.

INVITED LECTURE, WED./10:10

From mono- to polyhydroxyalcohols — how changes in molecular structure influence properties of the alcohols

S. Pawlus,¹ S. Kołodziej,² M. Wikarek,¹ M. Paluch¹

¹Institute of Physics, University of Silesia, Katowice, Poland

²Institute of Materials Science, University of Silesia, Katowice, Poland

Alcohols belong to group of associated liquids with very large number of representatives with different molecular structure architecture. It seems that the most important element of molecular structure, that mostly influence properties of these materials is position and number of hydroxyl groups (OH). However, also existence of some large enough pendant groups can markedly modified molecular dynamics of alcohols.

Studies of various alcohols with us of e.g. Broadband Dielectric Spectroscopy (BDS) provide unique possibility to better understand meaning of differences in molecular structure for properties of H-bonded liquids. However, not only changes of molecular architecture but also variation of thermodynamic conditions influence features of associated materials. During this presentation it will be showed how mentioned above factors: structure of molecules and changes of temperature and pressure are reflected by relaxation dynamics of alcohols.

Acknowledgement: The presentation financially supported by National Science Centre, Poland, Poject OPUS 9 (No.: UMO-2015/17/B/ST3/01221)

INVITED TALK, WED./10:40

Confinement-induced changes in molecular dynamics and crystallization behavior of isothiocyanatobiphenyl liquid crystals

M. Jasiurkowska-Delaporte,¹ E. Juszyńska-Gałązka,¹
P. M. Zieliński,¹ M. Marzec,² A. Baranowska-Korczyk³

¹Institute of Nuclear Physics Polish Academy of Sciences, Kraków, Poland

²Institute of Physics, Jagiellonian University, Kraków, Poland

³Faculty of Chemistry, University of Warsaw, Warsaw, Poland

Liquid crystals (LCs) enclosed in various porous systems have been intensively studied in recent years. It is already known that *hard* confinement imposed by the rigid pore walls induces new material features including optical properties, dynamic peculiarities and different phase diagram than in bulk. Other interesting, but as yet unexplored is *soft* confinement derived from the interactions between the polymer and guest liquid crystalline molecules. The purpose of this work is to exam the influence of different forms of spatial restrictions on molecular dynamics and crystallization behavior of 4-hexyl-4'-isothiocyanatobiphenyl (6BT) liquid crystal. Hard confinement was achieved by the infiltration of 6BT molecules into nanoporous aluminum oxide (AAO) templates with non-intersecting channels of mean diameters between 40 nm and 200 nm. Soft confinement was investigated on an example of electrospun polymer/liquid crystal composite fibers. We prepared composite fibers for three different mass ratios of polycaprolactone (PCL) and 6BT. By a combination of broadband dielectric spectroscopy and Fourier-Transform Infrared (FTIR), the microscopic picture of the influence of soft and hard confinement on molecular dynamics is obtained. In this talk, I will discuss similarities and differences in the impact of hard and soft confinement on dynamic properties and crystallization kinetics of 6BT liquid crystal.

Acknowledgements: M. J-D acknowledges the National Science Centre (Grant SONATA11: UMO-2016/21/D/ST3/01299) for financial support.

KEYNOTE LECTURE, WED./11:30

Design and synthesis of photomagnetic molecular sponges and site-selective photoswitchable clusters

D. Pinkowicz, M. Arczyński, M. Magott

Jagiellonian University, Faculty of Chemistry, Kraków, Poland

email: dawid.pinkowicz@uj.edu.pl

Photoswitching of the magnetization is an attractive functionality that can be incorporated into molecular crystals by following the design principles developed within supramolecular chemistry, crystal engineering and molecular magnetism. The extensive research of photomagnetic solids/molecules will eventually result in the construction of cutting-edge molecule-based devices: molecular sensors and switches.⁽¹⁾ Photomagnetism was observed for various classes of compounds: Prussian Blue analogues,⁽²⁾ valence tautomers⁽³⁾ or iron(II) spin crossover compounds.⁽⁴⁾ In the following communication two different groups of unique photomagnetic systems will be presented and discussed: photomagnetic sponges showing strong photo-induced magnetization depending on their hydration level (i) and photomagnetic cluster molecules comprising two photoswitchable centres responding differently to blue and red light (ii).

The photomagnetic molecular sponge systems are three-dimensional (3-D) coordination polymers based on paramagnetic metal centres that show reversible structural response to the sorption/desorption of the solvent molecules and a photomagnetic behavior that depends on the solvation level. The very first examples of such systems are strongly related to the magnetic sponges based on octacyanoniobate(IV).⁽⁵⁾ The compounds in question $\{[\text{Mn}^{\text{II}}(\text{imidazole})]_2[\text{W}^{\text{IV}}(\text{CN})_8]\}_n$ ⁽⁶⁾ and $\{[\text{Mn}^{\text{II}}(\text{imidazole})]_2[\text{Mo}^{\text{IV}}(\text{CN})_8]\}_n$ exhibit very high light-induced magnetic ordering temperatures and a magnetic hysteresis loop up to 90 K (the $[\text{W}^{\text{IV}}(\text{CN})_8]$ -based analogue) due to the light-induced excited spin state trapping (LIESST) phenomenon occurring at the $[\text{M}^{\text{IV}}(\text{CN})_8]$ -moiety.⁽⁷⁾ In both cases, the photomagnetic effect results from the blue light excitation (450 nm) of the constituent octacyanomethylate(IV) moieties, which then couple magnetically with manganese(II) inducing ferrimagnetic ordering.

The reported photomagnetic cages are hexanuclear bimetallic spin crossover (SCO) molecules $[\text{M}^{\text{II}}(\text{tmphen})_2]_4[\text{M}^{\text{IV}}(\text{CN})_8]_2\text{-solv}$ $\text{M}_4^{\text{II}}\text{M}_2^{\text{IV}}$ (tmphen=3,4,7,8-tetramethyl-1,10-phenanthroline; $\text{M}^{\text{II}}=\text{Fe}^{\text{II}}, \text{Mn}^{\text{II}}$; $\text{M}^{\text{IV}}=\text{Mo}^{\text{IV}}, \text{W}^{\text{IV}}$; solv=MeOH/H₂O) which are similar to their Nb-analogs.⁽⁸⁾ They adopt an octahedral geometry with the M^{IV} centres occupying apical positions and the M^{II} centres located in the equatorial plane. The Fe^{II} -based congeners Fe_4Mo_2 and Fe_4W_2 exhibit a gradual incomplete spin crossover behaviour while Mn_4Mo_2 and Mn_4W_2 are simple paramagnets. All four compounds exhibit exciting photomagnetic behaviour. Mn_4Mo_2 and Mn_4W_2 show a significant magnetization increase in response to violet/blue light due to the light-induced excited spin state trapping (LIESST) phenomenon occurring at the M^{IV} centres,⁽⁷⁾ while Fe_4Mo_2 and Fe_4W_2 are two-wavelength photomagnets that respond differently to red and violet light leading to a site-selective Fe^{II} - or combined $\text{Fe}^{\text{II}}\text{-Mo}^{\text{IV}}/\text{Fe}^{\text{II}}\text{-W}^{\text{IV}}$ LIESST effects, respectively.

Acknowledgments: This work was funded by the Polish National Science Centre within the Sonata Bis project No. 2016/22/E/ST5/00055.

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INVITED LECTURE, WED./12:10

Electronic transport through organic spin-containing molecules and their use for manipulating electronic properties of surfaces

J. Veciana

Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus de Bellaterra, Cerdanyola del Vallès, Spain
CIBER-BBN, Campus de la UAB, Bellaterra, Spain

Organic free radicals are neutral molecules exhibiting magnetic and optical properties due to the presence of an unpaired electron. This property together with their low spin-orbit couplings and weak hyperfine interactions make them good candidates for molecular spintronics insofar the radical character is preserved in solid state and the molecules are properly arranged on a solid state device. To exploit such properties we used functionalized polychlorinated triphenylmethyl (PTM) radicals to attach them as self-assembled monolayers (SAMs) on metallic surfaces, like Au, Ag, Cu, or graphene, exploring the transport properties through such spin-containing organic hybrid systems.⁽¹⁾ Also the transport through a single radical PTM molecules with two- (mechanically-controlled break junction) and three-terminal (electromigrated break junction) solid-state devices will be also reported.⁽²⁾ The magnetic property of radicals in these hybrid systems is manifested by the appearance of Kondo anomalies in the transport measurements. Also molecular junctions showing rectification properties will be reported.⁽³⁾ In all cases the conductance through the radical molecules is enhanced two orders of magnitude with respect the corresponding non-radical ones which can be explained by a mediated electron transport through the SUMO orbitals in the open-shell systems.^(4,5) These results paves the way towards the use of all-organic neutral radical molecules in spintronics.

In this contribution the use of such radical molecules for manipulate the electronic properties, like work function, of metallic surfaces will be presented showing that it is possible to prepare switch such electronic properties using external inputs like NIR light.^(6,7)

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INVITED TALK, WED./12:40

Multifunctional nanocomposites based on ordered mesoporous silica — synthesis and characterization

M. Laskowska, Ł. Laskowski

Institute of Nuclear Physics Polish Academy of Sciences, Kraków,
Poland

Ordered mesoporous silica matrices are widely used as a part of nanocomposites. Here we report such a composite composed of 2D hexagonally ordered mesoporous silica and metal ions, that are homogeneously anchored at the silica surface. In order to control the degree of functionalization and consequently the number of metal ions, the direct synthesis method (co-condensation) was used. In this case, the copper ions were covalently bonded to the silica matrix via propyl-phosphonate anchoring groups. Silica host matrices were prepared both in a form of powders and thin films, depending on the planned application. The copper-containing thin film material exhibits nonlinear properties and can be considered as a novel material for application in optoelectronic devices. Strongly dipolar propyl-copper-phosphonate units regularly distributed and anchored inside the silica matrix act as optically active centers. Additionally, the NLO susceptibilities can be tuned by tuning the degree of supramolecular interactions and also the molecular structure of the material by modification of the functional group concentration inside the matrix. Moreover, such a property of the copper-functionalized material can be boosted by utilizing additional silver-containing units.

The copper-containing nanocomposite showed also strong antibacterial action against *Escherichia coli* bacteria and appears to be a very promising material for a bactericidal application. Considering the properties of silica-based nanocomposites shown here, it can be concluded that this compounds family is a typical example of multifunctional materials.

INVITED TALK, WED./13:00

Using thin polymer film processing to obtain domains with Single Ion Magnets

A. Majcher,¹ M. Janik,¹ P. Dąbczyński,¹ M. M. Marzec,²
M. Ceglarska,¹ J. Rysz,¹ A. Bernasik,³ S. Ohkoshi,⁴
O. Stefańczyk⁴

¹Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University, Krakow, Poland

²Academic Centre for Materials and Nanotechnology, AGH University of Science and Technology, Kraków, Poland

³Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Kraków, Poland

⁴Department of Chemistry, School of Science, The University of Tokyo, Japan

Using a new approach to combine molecular magnetism and polymer science, we obtained a new material that combines merits of both these groups: Co(II)-based Single Ion Magnets exhibiting field-induced slow magnetic relaxations embedded in a polymer matrix (poly(4-vinylpyridine), P4VP), cross linking it. We also obtained a thin film of this material, preserving its qualities.⁽¹⁾ Taking this approach one step further, we used phase separation of polymer mixes to obtain domains that selectively adsorb CoBr₂, yielding functional domains that can be controlled by simple mass ratio of the polymers used in the mix. P4VP with polystyrene (PS), mixed in a common solution in various mass ratios were spun-cast onto silica substrates, self-organizing into phase-separated films with domains in sizes depending on the mass ratio. These films were then immersed in a solution of CoBr₂ in a solvent orthogonal for both polymers. While the P4VP domains, as shown previously, adsorbed the metal salt forming the aforementioned material, PS domains remained unaltered. All the films were characterized by Atomic Force Microscopy and Secondary Ion Mass Spectroscopy, confirming that we indeed obtained functional magnetic domains. Studies of the influence of magnetic field on domains topography will also be presented.

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CONTRIBUTED TALK, WED./13:20

Functionalization of MoS₂ with molecular-based systems: towards tuneable composites

I. Brotons,¹ E. Coronado,¹ A. Forment-Aliaga,¹ M. Giménez-Marqués,¹ M. Morant-Giner,¹ R. Torres-Cavanillas,¹ A. Alberola,¹ J. Dugay,¹ G. Escorcía,¹ M. Galbiati,¹ A. L. Gushchin,² J. Romero,¹ R. Sanchis-Gual,¹ N. Y. Shmelev,² S. Tatay¹

¹Instituto de Ciencia Molecular, Universitat de València, Paterna, Spain

²Nikolaev Institute of Inorganic Chemistry Siberian Branch of Russian Academy of Sciences, Novosibirsk, Russian Federation

Since the isolation of graphene in 2004, great efforts have been directed to the obtention of other two dimensional materials.⁽¹⁾ Among them, the so-called transition metal dichalcogenides (TMDCs), of general formula MX₂ (M: transition metal, X: chalcogenide), deserve special attention due to their broad spectrum of electronic properties arising from a large variety of compositions and polytypes.⁽²⁾

Nowadays, the preparation of multifunctional composites based on TMDCs and molecular materials is still a hot topic.⁽³⁾ Our work is focused on the covalent/electrostatic functionalization of MoS₂ with molecular systems (Figure 1) targeting two main goals:

a) Functionalization with systems that exhibit bistability controlled by external stimuli. Our idea is to be able to tune the intrinsic properties of the 2D material through the modulation of the molecular component. We have functionalized MoS₂ with spin crossover (SCO) nanoparticles.⁽⁴⁾ By changing an external stimulus, the SCO system changes its spin state along with other properties and this tunes the electronic structure of MoS₂.

b) Functionalization with molecular systems that improve the use of MoS₂ flakes for energy storage applications. In this way, we have functionalized MoS₂ with the coordination polymer Prussian blue (PB) giving rise to a new composite with outstanding behaviour as cathode for Na and K ion batteries.⁽⁵⁾ Furthermore, currently we are studying the electrochemical properties of a new composite (MoS₂ flakes decorated with a W cluster⁽⁶⁾), that could be used as a precursor of MoS₂/WS₂ heterostructures.

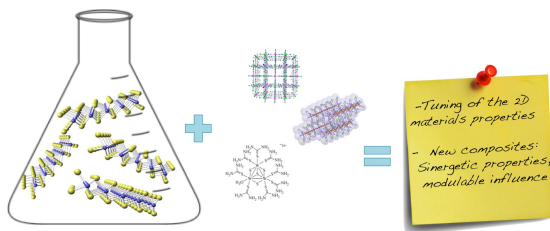


Figure 1. Schematic representation of chemically exfoliated MoS₂ flakes and the molecular based systems used in the present work.

Acknowledgements: M. Morant-Giner thanks the attendance grant for Multis2019 supported by Polish PROM program within the project *International scholarship exchange of the PhD students and academics*.

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KEYNOTE LECTURE, THU./09:00

Cubic phases formed by chain-core-chain type molecules — formation mechanism and molecular design

S. Kutsumizu

Department of Chemistry and Biomolecular Science, Gifu University,
Japan

The presence of cubic soft matter phases is now well recognized in various materials and living systems (block polymers, lipids, polysaccharides, etc.). Among them, thermotropic liquid crystalline (LC) systems are especially curious because a three-dimensional network structure is formed by the aggregation of one kind of molecule in fluid state, and in some case the chemical structure is not so much different from those of other molecules forming more conventional LC phases such as nematic or smectic phases. Our attention has been focused on such kind of relatively simple chain-core-chain type molecules that self-organize the cubic structures. In my presentation, the molecular organization and formation mechanism in two types of cubic phases, $Ia\bar{3}d$ -gyroid phase and a chiral cubic phase that was earlier recognized as $Im\bar{3}m$ symmetry are shown. Furthermore, the molecular design principle obtained is discussed. Here, I would like to stress that systematic but elaborate investigation with respect to the chain length and core size is effective to gain those insights.

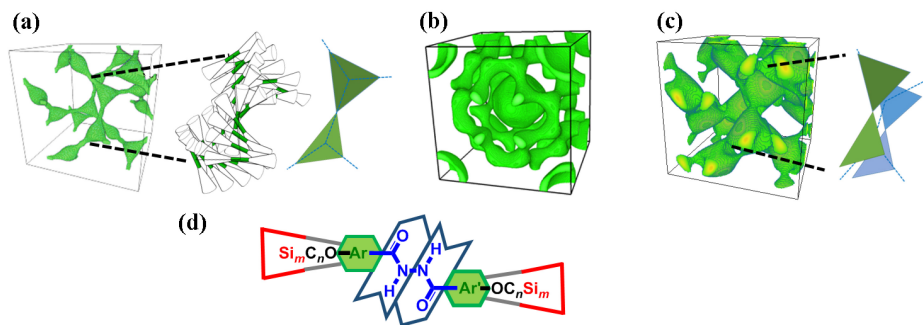


Figure 1. Molecular organizations for two types of cubic phases, (a, c) $Ia\bar{3}d$ -gyroid phase and (b) chiral cubic phase; (d) structural motif adopting an antispindle shape necessary for the formation of the cubic phases.

INVITED LECTURE, THU./09:40

Pinned solitons in genuine organic anion-radical salt (Et-2,6-diMe-Pz)(TCNQ)₂E. Čížmár,¹ D. Šoltésová,¹ P. Doležal,² D. Kriegner,³ M. Dušek,³
D. Ziolkovskiy,⁴ A. Feher¹¹P. J. Šafárik University, Institute of Physics, Košice, Slovakia²Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic³Institute of Physics of the Academy of Sciences of the Czech Republic, Prague, Czech Republic⁴V. N. Karazin Kharkiv National University, Department of Chemistry, Kharkiv, Ukraine

The crystal structure and magnetic properties of the new organic anion-radical salt (Et-2,6-diMe-Pz)(TCNQ)₂ were investigated. In the crystal structure of studied system the cation-containing layers alternate with layers where TCNQ anion-radical pairs carrying spin $S=1/2$ form stacks. A sudden decrease of the magnetic moment was observed at the temperature of 173 K and the observed transition is further accompanied by the appearance of a λ -anomaly in the temperature dependence of specific heat. Investigation of the crystal structure evolution across the transition temperature suggests the appearance of the spin-Peierls (sP) transition. The magnitude of the exchange coupling present in the high-temperature uniform chain structure ($J/k_B = 102$ K) and high sP temperature suggest that a phase transition of the second order appears in (Et-2,6-diMe-Pz)(TCNQ)₂. However, the studied system is unique due to its vicinity to the crossover point between the first-order and second-order type of transition that depends on the ratio of the magnetoelastic constant and exchange coupling.⁽¹⁾

Further EPR experiments below the sP transition revealed evidence of $S = 1/2$ species previously identified as pinned solitons. The dynamic susceptibility measurements also display a slow spin-lattice relaxation, which is a prerequisite for the observation of long quantum coherence time as observed in similar systems with pinned solitons.⁽²⁾ Due to the high spin-Peierls transition temperature, the studied system allows studying the spin dynamic of pinned solitons in a wide temperature range.

Acknowledgments: Supported by VEGA 1/0426/19 and VVGS-2019-1022.

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INVITED LECTURE, THU./10:10

Noble metal modified nickel electrodes for electrocatalysis

M. Oyama

Kyoto University, Japan

Metal nanoparticles (NPs) have been attracting active attention as functional units for electrode modifications because they can change the electronic communications on the conductive materials. If we would like to attach gold NPs (AuNPs) on the ITO surfaces, the functional bridging reagents such as (3-mercaptopropyl)-trimethoxysilane have been adopted. While many successful results have been obtained using the bridging reagents, our group proposed a simple methodology to attach AuNPs on the ITO surfaces. Namely, by applying a seed-mediated growth method to the surface modification, the crystal growth of AuNPs on the ITO surfaces could be performed from the Au nanoseed particles physically adsorbed on the ITO with keeping adhesion contacts. As the results, successful electroanalysis could be performed using thus prepared AuNP-attached ITO electrodes.

Although we utilized the absorption of Au nanoseed particles on Ni surface in the previous work, Au can be deposited on Ni surface using a very simple method. That is, because the oxidation potential of Ni to Ni ions is relatively negative, it is expected that Au deposits on Ni electrodes by the simple galvanic replacement reaction. When we use a wire of Ni as a base electrode, the modification of AuNPs was possible by just immersing a Ni wire into an aqueous solution of HAuCl_4 . The modified states of Au were evaluated by observing SEM images and cyclic voltammograms of H_2SO_4 , glucose etc. As the result, it was found that low concentrations of HAuCl_4 could change the electrochemical characteristics from those of a bare Ni wire electrodes.

Starting from the modification of Au on Ni wire electrodes, we explored the modification of Pd on Ni wire electrodes and Ni microparticles for applying the prepared nanocomposite materials to electrocatalysts, in particular, for ethanol oxidation in alkaline aqueous solutions. Furthermore, the modification of PdAu and PtAu on Ni wire electrodes have shown interesting promotion of the modification or deposition reactions. These progresses of the noble metals modification on Ni materials and their applications will be presented in the meeting.

Influence of nano-particle size on the properties of multiferroic TbMnO_3

A. Szytuła,¹ S. Baran,¹ W. Bażela,² M. Dul,² A. Hoser³

¹Institute of Physics, Jagellonian University, Kraków, Poland

²Institute of Physics, Cracow University of Technology, Poland

³Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

TbMnO_3 crystallize in the orthorhombic distorted perovskite crystal structure (space group $Pnma$). Magnetic and specific heat measurements indicate the change of magnetic properties at 7, 28 and 41 K.⁽¹⁾ Neutron diffraction data reveal sine modulated magnetic structure in both Tb and Mn sublattices at low temperatures and change of the Mn ordering from incommensurate to commensurate at 28 K. The transition at 28 K is accompanied by the increase of the polarization. Theoretical analysis indicates that the broken inversion symmetry creates a polar axis.

For the nano samples the magnetic data confirm the previous data, while the neutron diffraction data indicate the cluster-like character of the magnetic ordering in the Tb sublattice. Dielectric measurements confirm the existence of electric polarization below 28 K.⁽²⁾ The values of dielectric constant is reduced with increasing temperature of calcination.

An explanation of those can be done on the basis of thermal neutron diffraction data analysis of the parameters of the Mn-O bond. Obtained data concerning the Mn-O bond length, Mn-O-Mn bond angles, the Jahn-Teller parameter suggest that the nano-particle size plays an important role in modifying magnetic and dielectric properties of the studied material.

⁽¹⁾ T. Kimura, et al., Nature 426 (2003), 55.

⁽²⁾ S. Kharrazi, et al., Solid State Commun. 138 (2006), 395.

KEYNOTE LECTURE, THU./11:40

Mixed nano-oxides: interplay of intrinsic and substrate-induced effects

J. Goniakowski, C. Noguera

Institut des Nanosciences de Paris, CNRS and Sorbonne Université,
France

Ternary and mixed oxides represent promising materials for many applications because combining cations of different sizes and electronegativities can be used to tune the structural and electronic properties of the resulting oxide alloys. At the nano-scale, these properties are additionally impacted by an interplay of intrinsic (size and dimensionality) and substrate-induced effects, which may result in stabilization of oxide objects with unique characteristics, substantially different from those of their bulk counterparts. However, despite impressive advances in the fabrication, characterization, and control of metal supported oxide ultra-thin films and islands, a unified conceptual picture of the factors which drive the characteristics of cationic mixing at the nano-scale has not yet emerged.

In this context, considering the technological importance of transition metal oxides and in particular of M_2O_3 sesquioxides, we have considered a series of Au-supported $MM'O_3$ honeycomb monolayers ($M, M'=Ti, V, Cr, \text{ and } Fe$) and have analysed with help of first principle calculations the specificity of microscopic mechanisms behind their cationic mixing, as compared to these in the corresponding freestanding films and bulk materials.

INVITED LECTURE, THU./12:20

Ensemble sampling in materials research

P. T. Jochym, J. Łażewski

Department of Computational Materials Science, Institute of Nuclear Physics Polish Academy of Sciences, Kraków, Poland

Even the smallest systems in material science, including nanostructures, consist of large number of atoms. Furthermore, the configurational space for the system of even tens of atoms is very large and grows exponentially with the size of the structure. This fact prevents straightforward inclusion of all possible configurations in the calculation. Statistical mechanics teaches that many material properties and other phenomena (e.g. phase transitions, heat conductivity) are determined not by the detailed geometry of the particular atomic arrangement but by the properties of the statistical ensemble it is a member of. These properties could be investigated by statistical sampling of the ensemble. The presented results indicate that this technique may be used for derivation of mechanical properties of high-entropy systems. It turns out that even dynamical and non-linear properties of the system may be effectively investigated in this way. What is more, it allows for inclusion of temperature in the otherwise static calculations. We will demonstrate application of this technique to disordered and non-linear systems and describe its strengths, limitations and perspectives.

INVITED TALK, THU./12:50

The switching mechanism of finite and infinite chains of macrospins

D. Kuźma,¹ P. Sobieszczyk,¹ J. Kłós,² F. Montoncello,³
P. Zieliński¹

¹Institute of Nuclear Physics Polish Academy of Science, Kraków, Poland

²Faculty of Physics, Adam Mickiewicz University, Poznań, Poland

³Dipartimento di Fisica e Scienze della Terra, Università degli Studi di Ferrara, Italy

We study the transitions of low dimensional systems of macrospins between their equilibrium configurations under a uniform magnetic field and variations of their mutual distances. It is known that infinite equidistant chains in the antiferromagnetic configuration treated in the Stoner-Wohlfahrt model show no gap at the Brillouin zone border if the applied field vanishes. There is, therefore, no room for edge modes in this region in finite counterparts. A magnetic field and/or making every second distance of macrospins different results in the appearance of a band gap. Then bound states then occur as functions of the strength of the field. The bound states occurring below the lowest band of the bulk spin waves are essential in the switching mechanism from the antiferromagnetic to ferromagnetic configuration. The spin reversal is, namely, initiated by the bound mode localized at the macrospin polarized opposite to the applied field. The phenomenon is qualitatively different for odd and even number of macrospins in the chain. The transition from ferromagnetic to antiferromagnetic configuration does not occur under a uniform field without a thermal agitation. A hysteresis of ferromagnetic states is observed in its stead. We demonstrate that a differentiation of shapes and/or sizes of macrospins makes the recovery of the antiferromagnetic state possible without thermal fluctuations. The soft modes driving this kind of switching will be visualised.

CONTRIBUTED TALK, THU./13:10

Spatially correlated stochastic dynamics in self-assembly and glass transition

M. Majka

Jagiellonian University, Kraków, Poland

Stochastic, yet spatially correlated behavior occurs in a variety of physical systems, e.g. in plasma physics, micro-flows, ensembles of active particles and glassy dynamics. The Langevin equations driven by the Spatially Correlated Noise (SCN) are presented here as a framework to describe the collective molecular dynamics. The fluctuation-dissipation relation requires that SCN is accompanied by the collective dissipation, i.e. the multi-component friction matrix that depends on the inter-particle distances. This collective dissipation can encode a variety of effects, e.g. transient like-charge attraction and the reorganization of charge screening layer in ionic systems. It also predicts the glass-like transition, i.e. the SCN-induced rise in viscosity by the factor of 10^3 as the packing fraction of a system approaches certain critical value. The mechanism of this transition is fully analytically explainable and can be applied to the systems with arbitrarily chosen interactions. The cases of hard spheres and soft particles are discussed. Though differing from the physical glass transition in some aspects, this theory shows a direct causal relation between the presence of spatial correlations in thermal noise (which resembles dynamic heterogeneity) and the macroscopic rise in friction. The collective dissipation length, which diverges at the transition point, is also identified. As the nature of such divergent length-scale for glass transition is still under debate, this suggests a new possible approach to this problem.

INVITED LECTURE, THU./15:00

Neutron spectroscopy of single and entangled antiferromagnetic rings

T. Guidi

Rutherford Appleton Laboratory, ISIS, UK

email: tatiana.guidi@stfc.ac.uk

Molecular nanomagnets are model systems to study the spin dynamics and magnetic correlations in low dimensional magnets. Molecular wheels are a subclass of molecular magnets constituted by a finite number of magnetic ions at the vertices of regular polygons and interacting antiferromagnetically (AF). The advances in the chemical engineering of these molecules have allowed the synthesis of tailor-made systems displaying several interesting phenomena ranging from finite size effects on the magnetic properties of linear AF chains to the entanglement between complex spin systems. Neutron scattering techniques have been intensively and successfully used to study the microscopic properties of molecular magnets and have enabled to reveal the signatures of their quantum behaviour. I will show how inelastic neutron scattering experiments on single crystals of molecular rings can be used to directly determine the Fourier components of the two-spin dynamical correlations⁽¹⁾ and to portray entanglement in weakly coupled molecular qubits.⁽²⁾ Furthermore, polarized neutron diffraction experiments have been used to determine the local magnetization in finite antiferromagnetic chains and to reveal the finite size effects in their spin density distribution.⁽³⁾

⁽¹⁾ M. Baker, T. Guidi, et al., *Nature Physics* 8 (2012), 906.

⁽²⁾ E. Garlatti, T. Guidi, et al., *Nature Commun.* 8 (2017), 14543.

⁽³⁾ T. Guidi, et al., *Nature Commun.* 6 (2015), 7061.

INVITED LECTURE, THU./15:30

Magnetic interactions and spin dynamics of the multiferroic $(\text{NH}_4)_2\text{FeCl}_5(\text{H}_2\text{O})$

R. Fishman,¹ W. Tian,¹ J. Musfeldt,² J. Fernandez-Baca,¹
J. Singleton,³ J. H. Lee⁴

¹Oak Ridge National Laboratory, USA

²University of Tennessee, USA

³Oxford University, UK

⁴Ulsan National Institute of Science and Technology, South Korea

Molecule-based multiferroics are very sensitive to external pressures and fields due to their low energy scales, flexible molecular building blocks, and ease of cation substitution. The multiferroic behavior of any material sensitively depends on the microscopic interactions between the spins. We study the magnetic interactions in the multiferroic erythrosiderite $(\text{NH}_4)_2\text{FeCl}_5(\text{H}_2\text{O})$ based on first-principles calculations and an analysis of the inelastic neutron scattering (INS) spectra. In this material, a network of hydrogen bonds underlies a system of competing exchange interactions that creates a cycloidal spin state. Based on INS measurements on a single-crystal sample, we evaluate the magnetic interactions in this material and compare those predictions with first-principles calculations.

CONTRIBUTED TALK, THU./16:00

Magnetic properties of hybrid particles prepared by pulsed laser irradiation methods

Ż. Świątkowska-Warkocka,¹ T. Itina,² A. Pyatenko,³
N. Koshizaki,⁴ M. Marszałek¹

¹Institute of Nuclear Physics Polish Academy of Sciences, Kraków, Poland

²Laboratoire Hubert Curien, Saint-Étienne, France

³National Institute of Advanced Industrial Science and Technology, Japan

⁴Hokkaido University, Japan

Iron, cobalt or nickel and their oxide nanoparticles have received considerable attention due to their applications in magnetic, electronic, catalyst and biomedical purposes. Hybrid particles based on Fe, Ni, Co were prepared by a pulsed laser irradiation of colloidal nanoparticles dispersed in liquid. The sizes of particles, their morphology and composition were controlled by tuning the laser parameters, such as laser fluence, pulse duration, wavelength and/or irradiation time. Correlation between structure of obtained hybrid particles and their magnetic properties will be presented. Possible applications of obtained particles will be discussed.

POSTER N° 1., TUE./17:50

Study of the structure of titanium thin films deposited by e-beam PVD

J. Chojenka, M. Perzanowski, A. Zarzycki, M. Marszałek

Institute of Nuclear Physics Polish Academy of Sciences, Kraków,
Poland

Polycrystalline titanium thin films have been widely employed as interlayer between the substrate and coating in order to improve adhesion strength, corrosion resistance and wear performance, as well as to promote the growth of crystalline phases of the coating. At room temperature and ambient pressure, crystalline titanium has a hexagonal-close-packed lattice (α -Ti), however, at high temperature or high pressure it has body-centered-cubic structure (β -Ti) or hexagonal structure (ω -Ti), respectively. In this work, we show the face-centered cubic structure of Ti, not present in the $p(T)$ diagram of titanium. The Ti films were deposited by e-beam evaporation on monocrystalline silicon (100) wafers coated by gold layer of 100 nm thickness. Crystal structure was investigated by X-Ray Diffraction (XRD) and the presence of fcc phase was confirmed by Glancing Angle X-Ray Diffraction (GAXRD).

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POSTER N° 2., TUE./17:50

Zero-field magnetic susceptibility of molecular chain magnet Cu(II)-Fe(III) in the semiclassical model of isotropic chains

D. Czernia,¹ R. Pełka,¹ N. Tereba,² T. Muzioł,² R. Podgajny³¹Institute of Nuclear Physics Polish Academy of Sciences, Kraków, Poland²Faculty of Chemistry, Nicolaus Copernicus University, Toruń, Poland³Faculty of Chemistry, Jagiellonian University, Kraków, Poland

The development of new technologies requires constant searching for novel materials. One of the promising class of compounds are molecular magnets that have a unique feature of being multifunctional, i.e., they exhibit many interesting properties at the same time. These frequently unusual properties may find a potential application in spintronics, magnetic recording, magnetic refrigeration or magnetic sensing technology operated by light, pressure or humidity level.

It is often the case that molecular magnets display a low dimensionality of the coordination network and thus require special theoretical models to describe their physical properties adequately. Here, a semiclassical model⁽¹⁾ was used to analyse the magnetic susceptibility of a molecular magnet $[\text{Co}(\text{bpy})_2(\text{ox})][\text{Cu}_2\text{Fe}(\text{bpy})_2(\text{ox})_4] \cdot 8.5 \text{ H}_2\text{O}$ crystallizing in the monoclinic system (space group: $P21/c$), consisting of chains in which two Cu(II) ions carrying spin $1/2$ are alternately coupled with the Fe(III) ion with spin $5/2$.

In this approach, the magnetic structure comprises two coupled spin subsystems alternately arranged along a line. The first subsystem consists of a single high-spin paramagnetic ion while the other one is an arbitrary assembly of spin centres. While for the latter one a rigorously quantum approach must be taken, the former one may be treated classically. If the intramolecular couplings are isotropic, one can obtain an explicit formula for the zero-field magnetic susceptibility as a function of temperature.

The best fit of the theoretical prediction to the susceptibility data implies a strong antiferromagnetic exchange coupling between the Cu(II) ions together with a relatively weaker antiferromagnetic interaction between the Cu(II) and Fe(III) ions. The antiferromagnetic character of all the exchange couplings in the studied compound gives rise to a weak geometric frustration.

⁽¹⁾ J. Curély, R. Georges, Phys. Rev. B 46 (1992), 3520.

POSTER N° 3., TUE./17:50

Ternary Pt/Re/SnO₂/C system as an effective catalyst for application in fuel cells

E. Drzymała, G. Gruzeł, M. Parlińska-Wojtan

Institute of Nuclear Physics Polish Academy of Sciences, Kraków,
Poland

email: elzbieta.drzymala@ifj.edu.pl

One of the most challenging tasks of chemistry and physics is creating new, efficient and environment-friendly technologies for transforming chemical energy into electricity. An attractive alternative as an energy source became fuel cells fueled by ethanol. Unfortunately in most cases instead of carbon dioxide, which should be the main product of ethanol oxidation reaction (EOR), byproducts, which lower the overall efficiency of the fuel, are generated⁽¹⁾. Therefore, studies are often focused on the design and development of the appropriate type of catalysts, which could reduce the amount of unwanted byproducts. Currently the most effective catalyst for EOR, is the system composed from bimetallic platinum-rhodium alloy NPs, which are attached to larger tin dioxide NPs⁽²⁾. The high activity of this system is related to the fact that each of the three constituents plays its own important role in the oxidation pathway⁽³⁾. In the literature, also the crucial role of physical contact between metallic and oxide nanoparticles, is shown as fundamental for superior electrocatalytic performance^(2,4). In this work, instead of rhodium, rhenium was chosen. It facilitates the splitting of the C-C bond in ethanol and also weakens the bond strength between the Pt surface and products of partial ethanol oxidation such as CO, thereby reducing the blocking of the active Pt surface by intermediate products. The main aim of this study was to obtain a Pt/Re/SnO₂/C nanocatalyst in a controlled manner. For this purpose, the obtained individual NPs^(5,6) were assembled into ternary catalysts using intermolecular interactions. To ensure physical contact between individual NPs forming the catalyst system, zeta potential measurements were performed. The method proposed in this work led to the formation of the desired ternary NPs arrangement with physical contact between them, what was confirmed by scanning transmission electron microscopy (STEM) combined with energy dispersive X-ray spectroscopy (EDS) analysis⁽⁵⁾. X-ray diffraction (XRD) allowed to determine the catalyst structure and cyclic voltammetry (CV) allowed to investigate electrochemical properties in the perspective of their potential use as anode material in fuel cells fueled by ethanol. The obtained electrochemical results showed that the ternary Pt/Re/SnO₂/C nanocatalysts exhibit significantly higher efficiency towards ethanol oxidation reaction compared with the commercial platinum catalyst Pt from Tanaka.

Acknowledgments: Financial support from the Polish National Science Centre (NCN), grant UMO-2014/13/B/ST5/04497 is acknowledged.

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- (4) M. Parlinska-Wojtan, et al., *Appl. Catal., A: General* 570 (2019) 319-328.
- (5) E. Drzymała, et al., *J Nanoparticle Res.* 20 (2018) 144.
- (6) E. Drzymała, et al., *J. Phys. Chem. Solids* 107 (2017) 100-107.

POSTER N° 4., TUE./17:50

Magnetic properties study of iron oxide nanoparticles-loaded poly(ϵ -caprolactone) nanofibres

M. Fitta, M. Jasiurkowska-Delaporte, W. Sas, P. M. Zieliński

Institute of Nuclear Physics Polish Academy of Sciences, Kraków,
Poland

Nowadays, there is a strong industrial demand for materials with a high level of multi-functionality. Access to multi-functionality at the nanoscale requires the development of hybrid nanostructures that combine materials of different natures. One of the examples of such nanocomposites are polymers doped with inorganic magnetic nanoparticles. By combining magnetic and polymeric materials, composites with exceptional properties can be obtained. Thanks to this, they give a real chance for future applications in sensors, intelligent coatings or in medicine, where they are considered as targeted drug delivery systems as well as for cancer therapies

This work presents the synthesis and physicochemical characterization of the electrospun nanofibres of poly(ϵ -caprolactone) (PCL) doped by iron oxide nanoparticle with diameters of 5 nm. PCL is a semi-crystalline, hydrophilic polymer showing controllable biodegradation rates, biocompatibility, and flexible mechanical properties. In the composite material, two different concentrations of magnetic nanoparticles were used: 2 and 6 wt.%. PCL-based composites were investigated by means of scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR) and thermogravimetry (TGA). Special attention was paid on the analysis of magnetic properties, where we followed the evolution of changes in the magnetic behavior of the material depending on the concentration of magnetic nanoparticles.

POSTER N° 5., TUE./17:50

Dynamics and phase transitions in 1,2-cyclohexanediol and 1,3-cyclohexanediol isomers seen by calorimetric and dielectric spectroscopy methods

M. Gałązka,¹ M. Jasiurkowska-Delaporte,¹ M. E. S. Eusébio,²
M. T. S. Rosado,² E. Juszyńska-Gałązka,¹ E. Dryzek¹

¹Institute of Nuclear Physics Polish Academy of Sciences, Kraków, Poland

²CQC Departamento di Quimica, Universidade de Coimbra, Portugal

email: miroslaw.galazka@ifj.edu.pl

In recent years, a growth of organic crystals exhibiting specific preparation of compounds in various thermodynamic states have met with special interest as functions, sizes and structures of crystals play an important role in the production of a variety of devices and materials.^(1,2)

Cyclohexanediol isomers, despite the simplicity of their molecular structure, show a various solid state phase behaviour — from one crystal or plastic-crystal phase to several crystalline phases. For cis-1,3-cyclohexanediol (abbreviated as C13C), and trans-1,3-cyclohexanediol (abbreviated as T13C) isomers, differential scanning calorimetry (DSC), polarised light microscopy (POM), infrared spectroscopy (FT-IR), X-ray diffraction (XRD) measurements were carried out supported by the computational analysis.⁽³⁾ Whereas, adiabatic calorimetry, DSC, POM, FT-IR and XRD were used for study of cis-1,2-cyclohexanediol (abbreviated as C12C) and trans-1,2-cyclohexanediol (abbreviated as T12C).⁽⁴⁻⁷⁾ Isomers of C12C are used in the preparation of keto alcohols and polymers, they are a chiral auxiliaries in the synthesis of several enantiomeric pure compounds and are used in pharmacological and agrochemical industries⁽⁴⁾ and it was found in the scent gland of Canadian beaver.⁽⁸⁾

The results of Broadband Dielectric Spectroscopy and DSC of the trans and cis isomers of 1,2-cyclohexanediol and 1,3-cyclohexanediol will be presented. Numerical analysis of the dielectric spectra results points to complex dynamics of selected compounds in isotropic liquid, ordered crystalline and orientationally disordered (plastic) crystal phases. Two relaxation processes were found in plastic crystal phases in C12C and T13C. These processes are responsible for relaxation of free molecule and creating/breaking hydrogen bonds between molecules to forming clusters. One relaxation process was found in crystal phases and in isotropic liquid phase. Temperature dependences of mean relaxation times are of the Arrhenius type, except for T13C compound for which the Vogel-Fulcher-Tammann dependence is fitted. The electric conductivity, fitted by Jonscher power law, is of order as for semiconducting materials. An electrode polarisation of electrode effect is strong especially in isotropic liquid and in plastic crystal phases.

Acknowledgments: This work was supported by the Crystallize COST Action CM1402.

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POSTER N° 6., TUE./17:50

Synthesis and characterization of SnO₂@PtRhNi nanocatalysts for ethanol oxidation reaction

G. Gruzel,¹ P. Piekarz,¹ M. Pawlyta,² M. Parlińska-Wojtan¹

¹Institute of Nuclear Physics Polish Academy of Sciences, Kraków, Poland

²Institute of Engineering Materials and Biomaterials, Silesian University of Technology Gliwice, Poland

email: gruzel.grzegorz@gmail.com

Pt-based nanoframes seem to be the one of the most promising catalysts for many reactions, especially for oxidizing small organic molecules, such as ethanol. This is a crucial issue, due to the potential application of these nanoframes as catalysts in Direct Ethanol Fuel Cells (DEFC). The nanoframes have many advantages, among others, they provide many edges and corners, which are catalytically active due to the low coordination number of atoms on these edges and corners. Another advantage of the nanoframes is their high surface area to volume ratio, due to the removal of the non-functional atoms from the interior of nanoparticles. This operation not only improves the efficiency in catalytic reactions, but also minimizes the usage of precious metals such as platinum, rhodium, gold.

In present study, a novel PtRhNi nanoframes-based nanocatalysts is proposed for ethanol oxidation reaction (EOR). Moreover, in order to enhance the catalytic activity, the PtRhNi nanoframes are decorated with small SnO₂ nanoparticles. Herein, the synthesis route of the obtaining SnO₂@PtRhNi nanocatalysts is presented. First, the solid PtRhNi rhombic dodecahedral nanoparticles with PtRh-rich edges and Ni core were synthesized. Next, the Ni core was etched, which results in obtaining hollow PtRhNi nanoparticles. Subsequently, based on the zeta potential theory, PtRhNi nanoframes were decorated with SnO₂ nanoparticles. All nanostructures, i.e. solid PtRhNi and SnO₂ nanoparticles, PtRhNi nanoframes and SnO₂@PtRhNi heteroaggregates were characterized by STEM HAADF, EDS, ICP-OES and XRD techniques. The resulting SnO₂@PtRhNi heteroaggregates were deposited on high-surface area carbon and electrochemically tested, showing a 6 fold higher mass activity and 10 fold higher specific activity towards ethanol oxidation reaction than commercially available Pt catalysts. Excellent activity and durability make SnO₂@PtRhNi NPs a highly promising EOR anode electrocatalysts for DEFC.

POSTER N° 7., TUE./17:50

Polymorphism and light-induced spin transition in [Fe(Pm-*p*BrA)₂(NCS)₂]. Towards high T (LIESST)W. Guo,¹ N. Daro,¹ S. Pillet,² K. Chainok,¹ M. Marchivie,¹
G. Chastanet,¹ P. Guionneau¹¹CNRS, Univ. Bordeaux, ICMCB, France²Université de Lorraine, CNRS, CRM2, Nancy, France

email: wenbin.guo@icmcb.cnrs.fr

The Spin Cross Over (SCO) phenomenon is a change of the electronic configuration of a metal ion from the high-spin state (HS) to the low-spin state (LS) that can be induced by external stimulation, including thermal, light and pressure. Among them, light-induced excited spin-state trapping (LIESST) is usually observed only at low temperature. It is a great challenge to enhance the temperature of LIESST (T (LIESST)) towards higher temperature. T (LIESST) is greatly determined by the nature and the geometry of the inner coordination sphere, which can be strongly perturbed by structural motions and intermolecular interactions.^(1,2)

Two new polymorphs of mononuclear compound [Fe(Pm-*p*BrA)₂(NCS)₂] were designed and crystallized with Pm-*p*BrA=(4-Bromophenyl)-pyridine-2-ylmethylene-amine. Polymorphs A and B crystallizes in monoclinic space group with two independent crystallographic sites for Fe(II) in the asymmetric unit. A shows an abrupt hysteretic spin transition around 175 K and a high T (LIESST) at 110 K, probably one of the highest T (LIESST) in family of bidentate ligand. The crystal structure was investigated in the HS and LS states and also in the quenched HS* state showing that the spin-transition is associated to a reversible and large rotation of one part of the ligand. It also appears that the Fe(II) site shows a high distortion of the coordination sphere that could be related to the unusually high T (LIESST). On the contrary, polymorph B shows a gradual SCO without LIESST effect. The comparison of the variable temperature crystallographic investigations indicates clearly differences between the structural properties of A and B notably showing that the different magnetic behaviors originate from the ligand conformation modification during SCO. Furthermore, the close examination of the structure-properties relationships in A and B gives crucial indications for the design of high T (LIESST).

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POSTER N° 8., TUE./17:50

Slow magnetic relaxation in a gadolinium(III)-dioxophenanthroline qubit candidateG. Handzlik,¹ M. Magott,¹ F. Tuna,² A. M. Sheveleva,²
D. Pinkowicz¹¹Faculty of Chemistry, Jagiellonian University, Kraków, Poland²School of Chemistry and Photon Science Institute, The University of Manchester, UK

email: gabriela.handzlik@uj.edu.pl

Molecule-based magnetic systems are considered as good candidates for molecular qubits — quantum analogs of bits.⁽¹⁾ They show long-lived superposition of spin states with millisecond coherence times⁽²⁾ and offer unparalleled modification potential through chemical methods. Among different molecular qubit candidates, gadolinium(III) complexes seem to have certain advantages that make them also useful for the implementation of molecular qudits concept — an analog of a qubit with more than two accessible quantum states.

We report a series of isostructural $[\text{Ln}(\text{phendo})_4](\text{NO}_3)_3 \cdot x\text{MeOH}$ ($\text{Ln}=\text{Y}, \text{Gd}, \text{Tb}, \text{Dy}, \text{Ho}, \text{Er}, \text{Tm}, \text{Yb}$) complexes with a helicene-type 1,10-phenanthroline- N,N' -dioxide (phendo) ligand.⁽³⁾ The phendo-based ligand-scaffold enforces a strict C_4 symmetry on the Ln^{3+} ions in all complexes.

Magnetic measurements revealed that compounds based on Dy^{III} , Er^{III} and Yb^{III} exhibit slow relaxation of the magnetisation typical for Single Ion Magnets under an external DC field. Surprisingly, the Gd^{III} complex also shows similar behaviour. The pure undiluted compound relaxes slowly through two relaxation processes up to 3.5 K (AC magnetic susceptibility measurements in the 1 – 1000 Hz range). A solid state diamagnetic dilution of $[\text{Gd}(\text{phendo})_4](\text{NO}_3)_3 \cdot x\text{MeOH}$ with the Y^{III} analog ($\text{Gd}_{0.01}\text{Y}_{0.99}$ and $\text{Gd}_{0.003}\text{Y}_{0.997}$) results in the disappearance of the relaxation process related to the dipol-dipol interactions and the out-of-phase AC magnetic susceptibility maxima can be observed up to 4.9 K. Slow magnetic relaxation is also observed for frozen solutions of the Gd^{III} complex. Importantly, this type of slow magnetisation dynamics was previously observed only for a handful of Gd^{III} complexes.⁽⁴⁾ $[\text{Gd}(\text{phendo})_4](\text{NO}_3)_3 \cdot x\text{MeOH}$ doped into $[\text{Y}(\text{phendo})_4](\text{NO}_3)_3 \cdot x\text{MeOH}$ was also studied by means of pulsed EPR spectroscopy, which revealed that it shows coherent spin dynamics with the figure of merit $Q_M \approx 100$.⁽⁴⁾

Acknowledgements: This work was founded by the Polish Ministry of Science and Higher Education within the Diamond Grant (0191/DIA/2017/46) and the Polish National Science Center within Sonata Bis project (2016/22/E/ST5/00055).

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POSTER N° 9., TUE./17:50

Low temperature polymorphism and dynamic of lithocholic acid (LCA)

E. Juszyńska-Gałązka, W. Zając

Institute of Nuclear Physics Polish Academy of Sciences, Kraków,
Poland

A complex polymorphism and vibrational dynamics of lithocholic acid (3 α -hydroxy-5 β -cholanic acid) abbreviated as LCA, with molecular formula: C₂₄H₄₀O₃, have been studied by complementary computational and experimental methods. LCA has a steroid framework. It is one of the naturally occurring organic bile acids produced in the liver from cholesterol.⁽¹⁾ Thermal behaviour of pristine (never melted before)⁽²⁾ and after melting lithocholic acid was studied in a broad temperature range, from 20 K to 473 K, using several complementary methods. LCA is a good glass-former. The following phase transitions in LCA were established:

- for pure compound: Cr (464 K) — Is (during heating), and Is (363 K) — GIs (during cooling),⁽²⁾
- for compound after melting: gCr1 (145 K) — sCr1 (270 K) — Cr2 (heating up to 300 K) and after second re-heating Cr2 (275 K) — Is; were: GIs is a glass of isotropic liquid (Is), gCr1 — glass of crystal phase, sCr — supercooled crystal phase.

Hydrogen bonding promotes the formation of glassy states. The differences between the crystal phases and glassy state of LCA (pure and after melting), were shown and explained as resulting from a few networks of hydrogen bonds. Quantum chemical calculations indicated that lithocholic acid may exist in multimolecular systems connected by hydrogen bonds. Intermolecular interactions involve both a hydrophilic hydroxyl group and a polar carboxyl group. The presence of two hydroxyl groups strongly affects intermolecular interactions, as the steric structure of molecules leads to changes in the mentioned interactions. However, the physico-chemical properties observed for unmelted⁽³⁾ and melted LCA are different. Most likely, LCA in melt undergoes chemical dimerization, with a possibility of the formation of unstable short oligomers. This is what both the infrared absorption measurements and quantum chemical simulations seem to suggest.

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POSTER N° 10., TUE./17:50

Destructive influence of the edge dislocation on 4H-SiC properties — DFT study

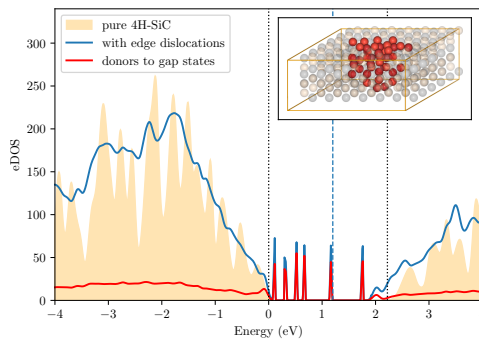
J. Łażewski, P. T. Jochym, P. Piekarz, M. Sternik, K. Parliński

Institute of Nuclear Physics Polish Academy of Sciences, Kraków, Poland

The silicon carbide (SiC), a wide band gap semiconductor, is a promising material for high-voltage and high frequency nanoelectronic devices. Its potential applications result from impressive value of breakdown voltage ($\approx 10^6$ V/cm), great charge carrier mobility, exceptional temperature stability and huge thermal conductivity. Additionally, it has very good mechanical properties and resistance to radiation damage. Unfortunately, the electronic properties of epitaxial layers strongly depend on the material's quality. The presence of intrinsic defects and impurities which arise during crystal growth process substantially limit applications of SiC. Dislocations are the main crystal defects in SiC. They deteriorate the performance of high electric field devices such as Shottky and *p-n* diodes.

Here, we present the ab initio study, based on density functional theory (DFT) methods, of full-core edge dislocation impact on basic properties of 4H-SiC semiconductor. To enable calculations in periodic boundary conditions we have proposed geometry with two dislocations with opposite Burgers vectors. The radial distribution function has been used to assess the effect of the dislocations on the local crystal structure. The analysis of the electronic structure reveals visible band gap narrowing and mid-gap *p* states appearance induced by broken atomic bonds in the dislocation core (see figure). The maps of charge distribution and electrostatic potential have been calculated and the significant decrease of the electrostatic barriers in the vicinity of the dislocation cores has been quantified.

This work was partially supported by the SICMAT Project financed under the European Funds for Regional Development (Contract No. UDA POIG.01.03.01-14-155/09).



POSTER N° 11., TUE./17:50

Mott criticality and glassy features of phonons induced by electron correlations in molecule-based superconductors studied by heat capacity measurements

Y. Matsumura,¹ S. Imajo,² S. Yamashita,¹ H. Akutsu,¹
Y. Nakazawa¹

¹Osaka University, Japan

²The Institute for Solid State Physics, The University of Tokyo, Japan

Thermodynamic discussion on the physical features around the two-dimensional Mott boundary of the dimer-Mott system of κ -type $(\text{BEDT-TTF})_2\text{X}$ system, where BEDT-TTF is bis(ethylenedithio)tetrathiafulvalene and X denotes monovalent counter anions is performed by systematic heat capacity measurements. $-(\text{BEDT-TTF})_2\text{X}$ is known to change its electronic ground state from Mott insulating state to superconductive one in accordance with the change the ratio of on-site Coulomb repulsion U and band width W . Since W is in proportion to the transfer integral t , it is tunable by the magnitude of external pressure. We used partially deuterated compounds of $-(\text{BEDT-TTF})_2\text{Cu}[\text{N}(\text{CN})_2]\text{Br}$ to pursue chemical pressure effect on thermodynamic properties. Systematic substitution by deuterons in the ethylene group of the BEDT-TTF donor induces slight contraction of molecular size and produces chemical pressure effect for the pristine compound located in the metallic/superconductive region ($T_c = 11.6$ K). With the increase of the number of deuteron in the molecules as is systematically described as $d[n, n]$ ($n = 0 - 4$), the position of the compound in the phase diagram shift to the Mott insulator side accordingly and crosses the boundary in the case of the $d[4,4]$ compound. We performed the heat capacity measurements of $d[2,2]$, $d[3,3]$, and $d[4,4]$ compounds in a temperature range of 1.0 – 50 K. The compounds of $d[2,2]$ and $d[3,3]$ located in the metallic region shows peculiar hump structure in the $C_p T^{-1}$ that is related to the glass-like features of phonons.⁽¹⁾ Since the system has a critical point in the phase boundary dominated by electron correlations as is suggested by Kagawa et al.,⁽²⁾ this glassy feature of phonons exist exceptionally in this region is considered as a supercritical mixing of the two phases as is typically observed in the liquid-gas boundary of water and CO_2 etc. We also report the thermodynamic peculiarity of the superconducting transitions near the Mott boundary using $d[2,2]$ and $d[3,3]$ compounds. Although the normal state γ term of these two compounds decreases due to the crossover from the Brinkmann-Rice region to Mott-Hubbard region as was reported in Ref. (3), the magnitude of the heat capacity jump at the transition temperatures seems to be enhanced which is something unexpected for partial superconductors. It is quite reasonable to consider that the electron correlations should be strong enough to make rigidly-coupled pairs in this region, but the stability of the band-like features which may be important to produce bulk superconductivity is much suppressed. We believe that the electronic properties of this region resemble the under doped region of the high- T_c oxides.

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POSTER N° 12., TUE./17:50

Exploring enhanced magnetocaloric effect in low dimensional magnets as potential refrigerants in high magnetic fields

M. W. Meisel,¹ M. Orendáč²¹Department of Physics and the National High Magnetic Field Laboratory (MagLab), University of Florida, Gainesville, USA²Institute of Physics, P. J. Šafárik University, Košice, Slovak Republic

email: meisel@phys.ufl.edu

In 2018, the 36 T, 40 mm bore Series Connected Hybrid (SCH) magnet became available.⁽¹⁾ In 2019, the first of a couple of 32 T, 34 mm bore All-Superconducting (AS) magnets⁽²⁾ is expected to be ready and equipped with a specialized dilution refrigerator system providing minimum lattice temperatures down to nominally 20 mK. These advances allow the possibility of pondering whether temperatures lower than typically available with dilution refrigerators can be achieved without using another magnet to adiabatically demagnetize a refrigerant like PrNi₅.⁽³⁾ This work explores one plausible avenue of exploiting the enhanced magnetocaloric effect of low dimensional antiferromagnets⁽⁴⁾ as a means of refrigerating samples by using part of the high field generated by the main magnet. Several groups have studied the large or enhanced magnetocaloric effect of different materials,⁽⁵⁻⁷⁾ and the present work considers possible options for adiabatic demagnetization refrigerants that employ other linear chain materials in fields near 30 T.

Acknowledgements: The National High Magnetic Field Laboratory (NHMFL or MagLab) is supported by the National Science Foundation (NSF) through DMR-1644779 and the State of Florida. This work was also supported, in part, by NSF DMR-1708410 (MWM), the Fulbright Commission (MWM, Scholar in 2013), and the Slovak National Funding Agency via APVV-14-0073 (MO).

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POSTER N° 13., TUE./17:50

Thermodynamic properties of organic conductors with charge fluctuation

T. Nomoto, S. Yamashita, H. Akutsu, Y. Nakazawa

Department of Chemistry, Graduate School of Science, Osaka University, Japan

In organic conductors composed by donor and acceptor molecules, it is possible to observe a lot of interesting physical phenomena derived from the strong correlation of itinerant electrons such as Mott insulating state, charge ordered state, superconductivity, and so on. In particular, in a system where geometrical frustration of donor arrangement exists, unique physical phenomena such as spin liquid, charge glass, and dipole liquid appear, and their origin and the application have been studied actively. In this study, we aimed to discuss the physical properties of organic conductors with pseudo two-dimensional triangular lattice by means of transport and thermodynamic measurement.

The organic conductor Θ -(BEDT-TTF)₂X series show a wide variety of electrical ground state from charge ordered insulating state to superconducting state. It is thought that the electronic ground state is changed due to the difference of counter cation X which changes the geometrical frustration of the system. Θ -(BEDT-TTF)₂I₃ which is closest to the regular triangular lattice change into the superconducting state at low temperatures. In contrast, Θ -(BEDT-TTF)₂CsZn(SCN)₄ which has the lattice close to the isosceles triangle shows a special electronic state called charge glass where the charge density is frozen inhomogeneously. In order to clarify the effect of charge frustration and fluctuation, we performed the thermodynamic measurement of Θ -type organic conductor systematically. The heat capacity and thermal conductivity measurement of Θ -(BEDTTTF)₂CsZn(SCN)₄ revealed that the strong coupling between the inhomogeneously fluctuating electrons and the lattice change the physical properties of lattice into structural-glass-like property. It can be said that this is a new glass formation mechanism driven by electron correlation. In the session, we will discuss the superconducting transition of Θ -(BEDT-TTF)₂I₃ and the effect of charge fluctuation in another donor arrangement.

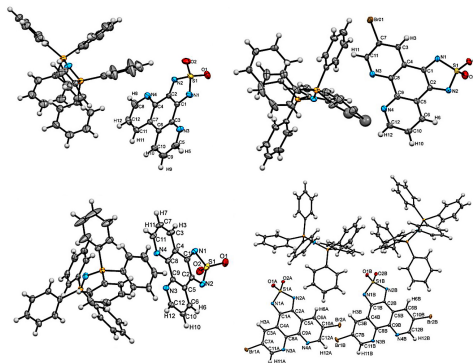
POSTER N° 14., TUE./17:50

Bis(triphenylphosphine)iminium salts of dioxothiadiazole radical anions

P. Pakulski, D. Pinkowicz, M. Arczyński

Jagiellonian University, Faculty of Chemistry, Kraków, Poland

Dioxothiadiazole moiety is a redox active function providing access to stable radicals suitable for the construction of molecular magnetic materials.⁽¹⁾ Phenanthroline-based systems can further be functionalized in order to tune the electronic and magnetic properties of those species. Bis(triphenylphosphine)iminium (PPN) salts of [1,2,5]thiadiazole[3,4-f][1,10]phenanthroline 1,1-dioxide, and its brominated analogues: 5-bromo-[1,2,5]thiadiazolo[3,4-f][1,10]phenanthroline 2,2-dioxide, and 5,10-dibromo-[1,2,5]thiadiazolo[3,4-f][1,10]phenanthroline 2,2-dioxide illustrate the impact of bromine substituents on crystal packing and magnetic properties of presented systems. PPN salt of [1,2,5]thiadiazole[3,4-f][4,7]phenanthroline 1,1-dioxide provides with an insight on how mentioned properties depend on the position of nitrogen atoms in the phenanthroline backbone. All PPN salts show antiferromagnetic interactions between the pairs of radical anions, which in the case of 5,10-dibromo analogue are very strong (-116 cm^{-1}) due to a different crystal packing of the anion radicals as compared to the rest of discussed derivatives.⁽²⁾



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POSTER N° 15., TUE./17:50

Mesomorphism and photochemistry of (E)-4-((4-octyloxyphenyl)diazenyl)phenyl alkanoates

M. Piwowarczyk,¹ N. Osiecka-Drewniak,¹ M. Gałazka,¹
Z. Galewski²

¹Institute of Nuclear Physics Polish Academy of Science, Kraków, Poland

²Faculty of Chemistry, University of Wrocław, Poland

email: marcin.piwowarczyk@ifj.edu.pl

Azobenzene derivatives in liquid crystals science are a very promising group of liquid crystalline compounds due to the ease of forming mesogenic phases as well as their light-sensitivity. This dual-functionality makes them extremely interesting materials for the challenges of modern physics. That is why it is so important to obtain new compounds of this kind.^(1,2)

In this work a new homologous series of (E)-4-((4-octyloxyphenyl)diazenyl)phenyl alkanoates was synthesized to check the effect of length growth of the hydrocarbon chain of the alkyl acid on the phase transition temperatures and the type of mesophases that occur (Fig.1). For all derivatives up to the octadecyl derivative the nematic phase was observed. From the pentyl derivative the smectic C phase occurred. From the propionic derivative all synthesized derivatives possess a smectic G phase. An additional extremely complex polymorphism of additional smectic phases was observed from the butyl to undecyl derivatives.

The influence of even-odd effect on the temperature of N-Iso phase transition is clearly visible. Although the behavior of the first two derivatives of the series is unusual. Thermal properties were obtained using DSC, TOA and POM method. Derivatives of this series absorb UV-Vis light causing trans-cis isomerization processes. Kinetic coefficients are typical for this class of compounds.

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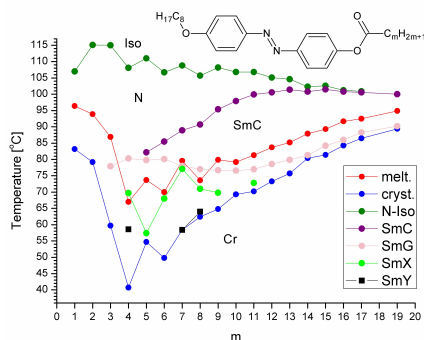


Figure 1. The phase situation of (E)-4-((4-octyloxyphenyl)diazenyl)phenyl alkanoates.

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POSTER N° 16., TUE./17:50

Formation of the Majorana bound states on defects

A. Ptok

Institute of Nuclear Physics Polish Academy of Sciences, Kraków,
Poland

Zero-energy Majorana bound states can emerge at the edge of a low dimensional systems.⁽¹⁾ Due to the Non-Abelian statistics of such states, Majoranas are a good candidate for the realization of qubit for topological quantum computer. However, if they are to be used in creation of quantum computer, it is crucial to obtain an intentional creation and manipulation of this type of bound states. We show such a possibility in a setup of several systems (e.g. optical trap⁽²⁾ or quantum dot-nanoring⁽³⁾ hybrid system) in which we artificially create a "defect" (inhomogeneity) region via electrostatic means. In such scenario, apart from non-trivial Majorana bound states, some trivial states like Andreev bound states can also be detected. We study the differences between those bound states and the possibility of their manipulation.

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POSTER N° 17., TUE./17:50

Self-assembled patterns of monolayer prepared on solid surface from DNA-CTMA complex

A. Radko,¹ J. Nizioł,² K. Makyła-Juzak,³ R. Ekiert,⁴ M. Marzec¹

¹Institute of Physics, Jagiellonian University, Kraków, Poland

²AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Kraków, Poland

³Department of General Chemistry, Faculty of Chemistry, Jagiellonian University, Kraków, Poland

⁴Department of Molecular Biophysics, Faculty of Biochemistry, Biophysics and Biotechnology Jagiellonian University, Kraków, Poland

Deoxyribonucleic acid (DNA) and its derivatives are a very interesting object of research due to their electrical properties. It seems that by controlling their properties, they can be used in molecular electronics.⁽¹⁾ Manipulation of natural DNA is impractical because it only dissolves in water.⁽²⁾ It is necessary to carry out modifications that will lead to new combinations of DNA with other chemical compounds forming complexes that will have desirable properties. One such combination is the DNA complex with hexadecyltrimethylammonium chloride⁽³⁾ (CTMA) cationic surfactant. The DNA-CTMA complex is insoluble in water but is soluble in a number of alcohols and some volatile non-polar solvents. In addition, it appears that the properties of the thin layer of the DNA-CTMA complex depend on the method and conditions of its preparation as well as on the type of DNA material used to form the complex.

The aim of this work is to study the topological differences of the monolayer of DNA-CTMA complex obtained by Langmuir-Blodgett technique (LB) using four different types of DNA: Low Molecular Weight DNA (LMW DNA), High Molecular Weight DNA (HMW DNA), plasmid DNA and short DNA obtained via Ion Exchange Chromatography technique from HMW DNA. Monolayers were deposited on two different substrates: hydrophilic mica and hydrophobic cleaned silicon wafer (Fig. 1). The properties of formed monolayers were studied by Atomic Force Microscopy (AFM) in non-contact mode at room temperature. Monolayers deposited onto silicon substrates did not show any organization while monolayers deposited onto mica formed organized structures dependent on DNA type, surface pressure as well as deposition rate.

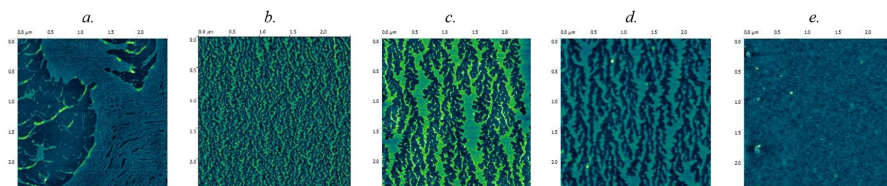


Figure 1. AFM images of thin layers of various DNA-CTMA complexes on mica slides: (a) plasmid DNA, (b) LMW DNA, (c) HMW DNA, (d) chromatography DNA and (e) chromatography DNA on silicon slide. Monolayers obtained by LB technique for surface pressure 15 mN/m and deposition rate 5 mm/min.

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POSTER N° 18., TUE./17:50

Structural and magnetic properties of Prussian blue analogue $\text{Fe}_3[\text{Cr}(\text{CN})_6]_2 \cdot n\text{H}_2\text{O}$ thin films obtained by electrodeposition and ion-exchange synthesis

W. Sas, M. Fitta

Institute of Nuclear Physics Polish Academy of Sciences, Kraków,
Poland

Molecular materials are getting more and more popular in recent years due to their unusual properties, which are not observed in traditional metallic magnetic materials. They can be characterized by a relatively high magnetic moment per unit of volume, low density, or sensitivity to external stimuli, such as temperature, light, or pressure. One of the best-known group of molecular magnets are Prussian blue analogues (PBAs), whose functional properties (photomagnetism, sorption capacity) are extensively studied.

This work presents synthesis and study of magnetic and structural properties of thin films based on hexacyanochromate, in particular, $\text{Fe}_3[\text{Cr}(\text{CN})_6]_2 \cdot n\text{H}_2\text{O}$. The samples were prepared on a transparent Nafion membrane by an ion-exchange process and on conducting PET-ITO foils by electrodeposition process. The surface pattern of both samples consists of a collection of nano- and microparticles, however some differences in their morphologies are observed. Some slight differences are also observed in magnetic properties. Both samples show sharp phase transition to a long-range ferromagnetically ordered state at $T_c = 20$ K and $T_c = 18$ K for the film deposited on PET-ITO and Nafion respectively.

POSTER N° 19., TUE./17:50

Magnetization reversal mechanism in nanopatterned multilayer with PMA and different antidots lattice symmetry

P. Sobieszczyk, M. Krupiński, P. Zieliński, M. Marszałek

Institute of Nuclear Physics Polish Academy of Sciences, Kraków, Poland

Fabrication and modeling of patterned thin films with perpendicular magnetic anisotropy rise great interest due to their wide applications in magnetic storage, sensors and magnonic crystals. A good representative of such systems are well-ordered arrays of magnetic antidots and dots based on Co/Pd multilayers, where magnetic reversal mechanisms strongly depend on the array geometry.^(1,2)

We attempt to understand and reproduce the observed magnetic properties and domain structure appearing in the hexagonal, quasiperiodic and randomly ordered arrays by micromagnetic simulations performed using Mumax3 software.⁽³⁾ In particular, changes in coercivity field, magnetic anisotropy constant and magnetic domain arrangement were studied and correlated with size and ordering, symmetry and size of nanostructures.

The domain pattern simulations shed light on the details of formation the Néel domain walls, as compared to Bloch walls, depends on the distances between the antidots. The calculations show how edge effects, defects and inhomogeneity affect magnetization reversal and domain wall pinning mechanism, which helps to design similar patterned systems with the specific magnetic properties.

Acknowledgments: The numerical simulations were supported in part by the PL-Grid Infrastructure.

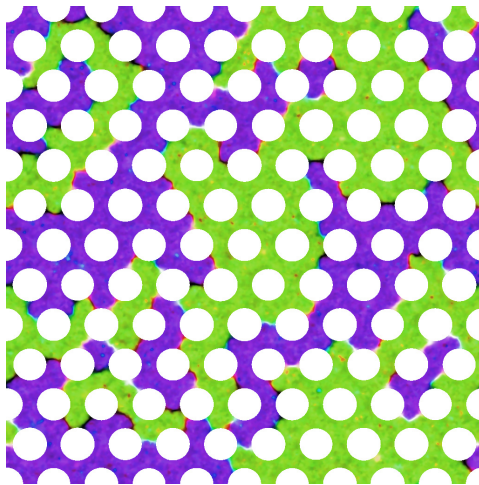


Figure 1. Simulated domain structure after ac demagnetization for the hexagonal lattice of antidots with diameter 140 nm.

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Ab initio and nuclear inelastic scattering studies of Fe₃Si/GaAs heterostructures

M. Sternik,¹ J. Kalt,² O. Sikora,¹ A. Ptok,¹ P. T. Jochym,¹
J. Łażewski,¹ K. Parliński,¹ P. Piekarz,¹ I. Sergueev,³
H.-C. Wille,³ J. Herfort,⁴ B. Jenichen,⁴ T. Baumbach,²
S. Stankov²

¹Institute of Nuclear Physics, Polish Academy of Sciences, Kraków, Poland

²Laboratory for Applications of Synchrotron Radiation, Karlsruhe Institute of Technology, Germany

³Deutsches Elektronen-Synchrotron, Germany

⁴Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The structure and dynamical properties of four variants of the Fe₃Si/GaAs(001) interface are investigated with density functional theory. We compare the stability of different configurations by calculating the formation energies and phonon dispersion curves. We present a comprehensive examination of charge density, magnetization, and electronic density of states. Our calculations unveil that magnetic moments of the Fe atoms tend to align in a plane parallel to the interface, along the [110] direction of the Fe₃Si crystallographic unit cell. In some configurations, the spin polarization of interface layers is larger than that of bulk Fe₃Si.

We discuss element-specific and layer-resolved phonon density of states in all variants. The Fe-partial phonon density of states measured for the Fe₃Si layer thickness of three monolayers is compared with theoretical predictions. The best agreement is found for one of the configurations with a mixed Fe-Si interface layer, which reproduces the anomalous enhancement of the phonon density of states below 10 meV.

POSTER N° 21., TUE./17:50

Thermal instability of carbamazepine

A. Dołęga, P. M. Zieliński

Institute of Nuclear Physics Polish Academy of Sciences, Kraków,
Poland

email: pm.zielinski@ifj.edu.pl

Carbamazepine (CBZ), an active pharmaceutical ingredient (API) commonly used in the treatment of epilepsy, mental disorders and neuropathic pain, exhibits low solubility and high permeability (BCS Class II). Four polymorphic forms of CBZ were characterized so far,⁽¹⁾ with melting point of the most thermally stable one (Form I) reaching 192°C while the decomposition temperature of the compound was reported to be 227°C.⁽²⁾

In course of experimental research concerning improvement of low bioavailability we have observed unusual thermal behaviour of CBZ during subsequent heating cooling cycles.⁽³⁾ The results of DSC, TGA and HS-POM (Hot-Stage Polarized Optical Microscopy) measurements showed that cooled from isotropic liquid phase at the rate 10°C min⁻¹ or higher CBZ totally vitrifies while cooling at the rate of 5°C min⁻¹ leads to partial crystallization and vitrification. Moreover CBZ tends to form amorphous state due to it is thermal instability at higher temperatures, namely decomposition of the compound starting already below melting point of Form I, that is more than 30°C lower than reported in the literature so far. We have also showed that obtained amorphous state is not pure glass of CBZ but a mixture of CBZ and iminostilbene. To the best of our knowledge our work (3) is the first one reporting instability of CBZ below melting temperature of Form I.

Acknowledgments: AD has been partly supported by the EU Project POWR.03.02.00-00-I004/16

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POSTER N° 22., TUE./17:50

Automatic apparatus for studying the sorption properties of intermetallic compounds

M. Żurek,¹ A. Budziak,¹ A. Dębski²

¹Institute of Nuclear Physics Polish Academy of Sciences, Kraków, Poland

²Institute of Metallurgy and Materials Science Polish Academy of Sciences, Kraków, Poland

Hydrogen is one of the most promising, future energy carriers. When hydrogen is burned directly, nitrogen oxides and water vapor are produced, while when hydrogen is oxidised in the fuel cells, the by-product is only water vapor. The energy produced from hydrogen belongs to one of the purest methods of energy production and at the same time is inexhaustible. Hydrogen can be produced from fossil fuels (natural gas, oil and coal) as well as in the electrolysis of water. The method of obtaining hydrogen in fermentation processes with the participation of appropriate bacterial strains is also very promising.⁽¹⁾ The nutrient medium for bacteria may be organic waste from the sugar industry or municipal waste. Although the latter method is very pro-ecological, it has its disadvantage. The fermentation products, in addition to hydrogen, are also CO₂/CO or hydrogen sulphide. This is a major obstacle to the efficient storage of hydrogen in metallic compounds. Contaminants can be removed to a large extent, but in some cases even traces of them can be important. Modification of compounds like LaNi₅ toward ternary compositions change alloy hydrogen storage properties and influence resistance to hydrogen contamination.⁽²⁾ In order to investigate the effect of contaminated hydrogen on the sorption storage of AB₅ type metallic compounds (mainly based on LaNi₅), an automatic sorption apparatus was constructed whose operation is based on the Sieverts volumetric method. The schematic diagram of the apparatus, the actual appearance and the first sorption results for compounds LaNi_{5-x}M_x (M: metal) treated with H₂ and CO₂ (with different concentrations) will be presented. In addition, structural and thermodynamic results (*cpT*) will be presented.

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MONDAY/01.07		TUESDAY/02.07		WEDNESDAY/03.07		THURSDAY/04.07	
12:00-15:00	registration	SOFT MATTER & APPLIED PHYSICS		09:00	MARIAN PALUCH	09:00	VLADIMIR NOVIKOV
				09:40	MALGORZATA ŚLIWIŃSKA-BARTKOWIAK	09:40	THOMAS BLOCHOWICZ
15:10	TOM LANCASTER	NANOMAGNETS, NANOSTRUCTURES, CONDUCORS		10:10	WYCLIFFE KIPROP KIPNUSU	10:10	SEBASTIAN PAWLUS
				10:40	HAL SUZUKI	10:40	M. JASURKOWSKA-DELAPORTE
16:10	welcome party	MULTIFUNCTIONAL MATERIALS & APPLIED PHYSICS		11:00	LUKASZ KOLEK	11:00	coffee break
				11:20	coffee break	11:30	DAWID PINKOWICZ
15:00	opening	MULTIFUNCTIONAL MATERIALS & APPLIED PHYSICS		11:50	EVA PAVARINI	12:10	JAUME VEGLANA
				12:30	ATSUSHI KAWAMOTO	12:40	MAGDALENA LASKOWSKA
15:00	TOM LANCASTER	MULTIFUNCTIONAL MATERIALS & APPLIED PHYSICS		13:00	YASUHIRO NAKAZAWA	13:00	ANNA MAJCHER
				13:20	MICHAŁ KRUPIŃSKI	13:20	MARC MORANT-GINER
15:00	TOM LANCASTER	MULTIFUNCTIONAL MATERIALS & APPLIED PHYSICS		13:40-15:00	lunch break	13:40-15:00	lunch break
				15:00	SILVIA BORSACCHI	15:00	TATIANA GUIDI
16:10	welcome party	MULTIFUNCTIONAL MATERIALS & APPLIED PHYSICS		15:30	ALEKSANDRA PAIZDERSKA	15:30	RANDY FISHMAN
				16:00	CHRISTOPHER STANTON	16:00	Ż. ŚWIĄTKOWSKA-WARKOCKA
16:10	welcome party	MULTIFUNCTIONAL MATERIALS & APPLIED PHYSICS		16:20	MARCO GEPPI	16:20	closing
				16:40	TETIANA NAGORNA	16:20	closing
16:10	welcome party	MULTIFUNCTIONAL MATERIALS & APPLIED PHYSICS		17:05	AGNIESZKA DOŁĘGA	excursion & conference dinner	
				17:15	WENBIN GUO		
17:25	OLEKSANDR PASTUKH						
17:35	MICHAŁ ŻUREK						
16:10	welcome party	MULTIFUNCTIONAL MATERIALS & APPLIED PHYSICS		17:50-19:45	POSTER SESSION	excursion & conference dinner	
				conference communications (7+3 min)			