Šiuolaikinės kietojo kūno BMR ir sukinių dinamikos tendencijos: link nedestruktyviųjų agentų peptidų pagrindu dinaminei branduolių polarizacijai (DNP)

Modern trends in solid-state NMR and spin dynamics: towards peptide based non-destructive polarizing agents for dynamic nuclear polarization (DNP)

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Joint Chemical Physics Seminar and Project Meeting,

Vilnius, October 11, 2018

Faculty of Physics, Saulėtekio alėja 9, building 3, Auditorium 401

Program

13:00 - 13:45

Dr Torsten Gutmann (TU Darmstadt)

Structural insights on functional materials and catalysts by DNP enhanced solid state NMR

The presentation will give an overview on recent advances on the characterization of functional materials and heterogeneous catalysts by solid-state dynamic nuclear polarization (solid-state DNP). The solid-state DNP approach is briefly introduced and its application for structure determination of multicomponent materials based on cellulose and polymers is presented. Furthermore, it is shown how this approach can be applied to heterogenized transition metal catalysts to obtain information on surface sites and the structure reactivity relationship.

Coffee break (15 min)

14:00 - 14:45

Dr Vytautas Klimavicius (TU Darmstadt), Alexander von Humboldt fellow

Spin dynamics and application of novel biradicals in surface enhanced DNP spectroscopy

The presentation will be mainly based on the systematic investigation of new type of biradicals for the purpose to use them in DNP spectroscopy. The newly reported polarization transfer mechanism will be discussed. Moreover, the application of surface enhanced DNP spectroscopy in studying 'real world' systems, namely supported nano-scale noble metal catalysts, will be presented.

Coffee break (15 min)

15:00 - 16:00

Prof Dr Vytautas Balevicius (Vilnius University)

Quasi-equilibria and polarization transfer between adjacent and remote spins: Glycine powder

The models of isotropic and anisotropic spin-diffusion are improper to describe the cross polarization (CP MAS) kinetics in the system with remote spins. The essential improvement of existing models was achieved taking into account the thermal equilibration in the reservoir of the abundant spins (^{1}H) after the polarization has been transferred. The treatment was demonstrated on powdered sample of glycine.

Glycine is the smallest and the second most widespread member of the amino acid family, found in proteins, enzymes and hormones and functions as a neurotransmitters. Also the collagen, which contains glycine at every third position in the peptide chain, has to be noted. It is present in bones and plays an important role in biomineralization processes.

As glycine is the smallest and simplest member in the series of amino acids, it is a good model compound proving the treatment of CP, namely - local order effects and spin thermodynamics. In future such processing can be applied for the whole series of amino acids.

Discussions: Further perspectives of collaboration between Vilnius and Darmstadt Universities

Closing

Scientists and students interested in Material Science, Life- and Chemical Physics are very welcome!