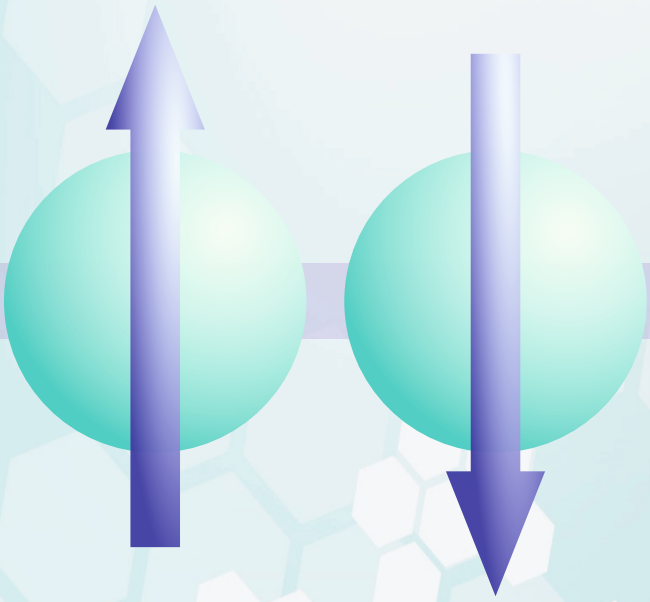
IV International School for Young Scientists

Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics

September 4-8, 2016, Akademgorodok, Novosibirsk, Russia

Book of Abstracts



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IV International School for Young Scientists ‘Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics’

September 4-8, 2016, Akademgorodok, Novosibirsk, Russia

IV International School for Young Scientists "*Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics*" will be held on September 4-8, 2016 in the Akademgorodok (Academy town) of Novosibirsk, Russia. Students, PhD students and young scientists from various fields of magnetic resonance will participate in the School. The program will include instructional lectures, oral talks by young scientists, poster sessions and practical tutorials on modern EPR and NMR spectrometers. As the School grows into maturity and former students themselves become active researchers, some instructional lectures will be delivered by young researchers and faculty to promote the continuity of scientific generations. We cordially welcome all the participants and guests in Akademgorodok this September to share their knowledge, expertise and passion for science with the younger generation of NMR/EPR people.

Official language of the School will be English. Scientific sessions will be held at the Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, tutorials will be organized in the research laboratories of the institutes of Akademgorodok. ‘Best oral talk’ and ‘Best poster’ competitions will be held and the winners will be duly acknowledged.

Scope

- Active sites in heterogeneous catalysis
- Basics of magnetic resonance
- Magnetic resonance imaging in physics, chemistry, biology and medicine
- Magnetic resonance for in situ studies in chemistry and material science
- Molecular magnets and supramolecular systems
- Paramagnetic states in functional materials and nanostructures
- Quantum chemistry in magnetic resonance applications
- Solid state magnetic resonance
- Spin chemistry
- Spin manipulation and quantum computing by magnetic resonance methods
- Synthesis, properties and applications of spin probes and labels

Organizers

- Voevodsky Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Sciences (ICKC SB RAS)
- International Tomography Center, Siberian Branch of Russian Academy of Sciences (ITC SB RAS)
- Novosibirsk State University (NSU)
- Siberian Branch of the Russian Academy of Sciences (SB RAS)

Supported by

- Russian Foundation for Basic Research

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The influence of spin-diffusion effect in conformational analysis of small molecules by 2D NOESY

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Two-dimensional Nuclear Overhauser Effect Spectroscopy (2D NOESY) is applied to the investigation of conformational equilibrium and chemical structure of small flexible molecules in a liquid phase system. An important influence of spin diffusion effect on the 2D NOESY-based analysis of conformational equilibrium for small flexible molecules in liquid was discovered. Therefore, the spin diffusion should be eliminated from the obtained 2D NOESY data in order to obtain accurate results. All widely applied approaches for spin diffusion suppression were critically analyzed, and two powerful approaches were tested for small flexible molecule. 2D Quenching Undesirable Indirect External Trouble in Nuclear Overhauser Effect Spectroscopy (QUIET-NOESY) with selective Q3 pulse was found to be a usefully approach to solve the problem of spin-diffusion effect. An alternative way to solve this problem, a combined analysis of two different NMR methods, 2D NOESY and two-dimensional Transverse Rotating-frame Overhauser Enhancement Spectroscopy (T-ROESY), was evaluated and proved to be the most correct way of obtaining conformer fractions for a flexible molecule in liquid.

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