PHYSICAL AND TECHNOLOGICAL SCIENCES

Magnetic resonance spectroscopy group

Keywords: *NMR of advanced materials in solid and liquid states; CW-FT EPR spectroscopy*

Vilnius University

Research group activities

- Crystallographic aspects, spin diffusion and spin-clusters size profile determination in nano-structured complex solids applying CP-MAS technique;
- Structure elucidation of organic compounds applying high resolution 1D/2D NMR techniques;
- Molecular-ionic processes in ionic liquids and composites forming liquid crystalline iono-gel mesophases;
- Large-amplitude proton dynamics in hydrogen bonded systems;
- EPR Studies of defects induced by (I) impurities; (II) by ionizing radiation: (III) free radicals in bio-systems.

Proposal

NMR spectroscopy of solids and liquids:

Magic angle spinning (up to 15 kHz) experiments for solid state NMR with 400 MHz wide bore magnets. The probe possesses an X channel which is tunable from 15N to 31P. Wide line NMR experiments – starting from polymers to single crystal studies and metal physics in frequency range 109Ag – 31P; Variable temperature range –150°C to +400°C; Static low temperature wide line NMR applications for 109Ag – 31P; Variable temperature range from room temperature to > 8K.

EPR spectroscopy:

CW regime: sensitivity: weak pitch international standard 2500:1; absolute 1.2 x 109 spins / G; up to 80 MHz tuning range; FT regime: sensitivity: with 10 µM TEMPOL in toluene in 10 sec 200:1; 2 ns time pulse resolution. Helium Temperature Control System (3.8 - 300 K); Variable Nitrogen Temperature Control System (Temperature range 100 K - 500 K); Programmable one axis goniometer, 1/8 degree resolution.

Meet our team

Lead researcher

Prof. Habil. Dr. **Vytautas Balevičius**

Team members

Prof. Habil. Dr. **Jūras Banys**

Dr. **Vidmantas Kalendra**

Dr. **Vytautas Klimavičius**

Dr. **Arūnas Maršalka**

PhD Students

Mantas Šimėnas

Laurynas Dagys

Research outcomes

Most important publications

- **Balevicius V., Aidas K., Svoboda I., and Fuess H.**, Hydrogen bonding in pyridine N-oxide/acid systems: proton transfer and fine details revealed by FTIR, NMR and X-ray diffraction. – J. Phys. Chem. A, 2012, v.116, p. 8753-8761;
- **Klimavicius V., Gdaniec, Z., Kausteklis, J., Aleksa, V., Aidas, K., and Balevicius, V.**, NMR and Raman Spectroscopy Monitoring of Proton/Deuteron Exchange in Aqueous Solutions of Ionic Liquids Forming Hydrogen Bond: A Role Of Anions, Self-Aggregation, and Mesophase Formation. – J. Phys. Chem. B, 2013, v.117, p. 10211-10220;
- **Klimavicius V., Kareiva A., and Balevicius V.**, Solid-State NMR Study of Hydroxyapatite Containing Amorphous Phosphate Phase and Nano-Structured Hydroxyapatite: Cut-Off Averaging of CP MAS Kinetics and Size Profiles of Spin Clusters. - J. Phys. Chem. C, 2014, v.118, p. 28914-28921;
- **Klimavicius V., Dagys L., and Balevicius V.**, Subnanoscale Order and Spin Diffusion in Complex Solids through the Processing of Cross-Polarization Kinetics. - J. Phys. Chem. C, 2016, v.120, p. 3542-3549;
- **Dagys L., Klimavicius V., and Balevicius V.**, Processing of CP MAS kinetics: Towards NMR crystallography for complex solids. - J. Chem. Phys. 2016, v.145, 114202 (9).

Resources

Bruker AVANCE 400 WB and Bruker AVANCE 400 SB spectrometers. Frequency 400 MHz, 2 superconducting magnets of wide- and standard bore, electronic units for independent (parallel) NMR investigation of solid and liquid state.

Bruker X-Band CW/FT EPR Elexys 580 spectrometer, working in pulse FT and CW regimes.

Contacts

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