



Monday 03rd September 2018
12.00h CIC energigUNE
Seminar room

Host:
Dr. Juan Miguel López del Amo

Seminar: “From NMR of noncovalent interactions to the local structural features of solids”



Speaker:
Dr. I. G. Shenderovich

From:
Faculty of Chem. and Pharm.,
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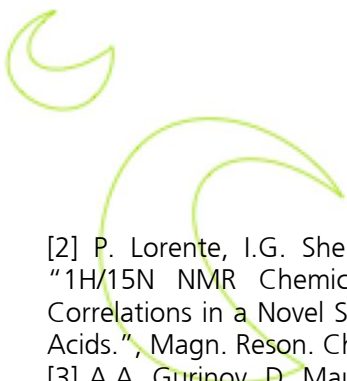
The mechanical and chemical properties of solids depend on their morphology. There are many methods designed to determine the composition of very complex materials. There is a lack of methods suitable to study intermolecular interactions and associated local structural features even into simple noncrystalline solids. Magnetic resonance spectroscopy (NMR) is the method of choice for such applications. The only critical requirement of NMR is the presence in the system of interest of spin-labels that can provide solutions of problems under consideration.

This presentation will cover the following aspects:

- (i) What nuclei can serve as most suitable spin-labels?
- (ii) How noncovalent interactions affect NMR parameters? [1,2]
- (iii) What one can learn about the morphology of surfaces using solid-state NMR? [3-5]
- (iv) Time-efficient DFT calculations as a complement to solid-state NMR. [1,6]
- (v) Reconstruction of the morphology of noncrystalline organic solids from NMR parameters of spin-labels. [7,8]

References

[1] I.G. Shenderovich, “Effect of Non-Covalent Interactions on the ^{31}P Chemical Shift Tensor of Phosphine Oxides, Phosphinic, Phosphonic, and Phosphoric Acids and Their Complexes with Lead(II).”, *J. Phys. Chem. C*. 2013, 117, 26689–26702.



- [2] P. Lorente, I.G. Shenderovich, N.S. Golubev, G.S. Denisov, G. Buntkowsky G., H.-H. Limbach, "1H/15N NMR Chemical Shielding, Dipolar 15N,2H Coupling and Hydrogen Bond Geometry Correlations in a Novel Series of Hydrogen-Bonded Acid-Base Complexes of Collidine with Carboxylic Acids.", *Magn. Reson. Chem.* 2001, 39, S18-S29.
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- [4] D. Mauder, D. Akcakayiran, S.B. Lesnichin, G.H. Findenegg, I.G. Shenderovich, "Acidity of Sulfonic and Phosphonic Acid-Functionalized SBA-15 under Almost Water-Free Conditions.", *J. Phys. Chem. C* 2009, 113, 19185-19192.
- [5] I.G. Shenderovich, G. Buntkowsky, A. Schreiber, E. Gedat, S. Sharif, J. Albrecht, N.S. Golubev, G.H. Findenegg, H.-H. Limbach, "Pyridine-15N - a Mobile NMR Sensor for Surface Acidity and Surface Defects of Mesoporous Silica.", *J. Phys. Chem. B.* 2003, 107, 11924-11939.
- [6] I. G. Shenderovich, "Simplified Calculation Approaches Designed to Reproduce the Geometry of Hydrogen Bonds in Molecular Complexes in Aprotic Solvents.", *J. Chem. Phys.* 2018, 148, 124313.
- [7] G.U. Begimova, E.Yu. Tupikina, V.K. Yu, G.S. Denisov, M. Bodensteiner, I.G. Shenderovich, "Effect of Hydrogen Bonding to Water on the 31P Chemical Shift Tensor of Phenyl- and Trialkylphosphine Oxides and α -Amino Phosphonates.", *J. Phys. Chem. C.* 2016, 120, 8717-8729.
- [8] R. Manriquez, F.A. Lopez-Dellamary, J. Frydel, T. Emmler, H. Breitzke, G. Buntkowsky, H.-H. Limbach, I.G. Shenderovich, "Solid-State NMR Studies of Aminocarboxylic Salt Bridges in L-Lysine Modified Cellulose", *J. Phys. Chem. B* 2009, 113, 934-940.