PHYSICAL AND TECHNOLOGICAL SCIENCES

Theoretical Spectroscopy Group

Vilnius University

Keywords: *molecular modelling, molecular dynamics simulations, quantum chemistry, density functional theory, QM/MM methods, NMR spectroscopy, UV/VIS absorption, charge transfer, charge redistribution processes, aqueous acidity constants.*

Research group activities

The main focus of our research is on the following fields:

- Modelling of quadrupolar NMR relaxation of monoatomic ions using molecular dynamics simulations as well as advanced quantum mechanics/molecular mechanics approaches
- Development of new computational schemes for reliable predictions of aqueous acidity constants of drug-like molecules
- Rational design of molecular compounds possessing favourable electronic properties for nanorobotics, toxic material recognition and long-lived molecular transistors

Spectroscopic parameters governing quadrupolar NMR relaxation of monoatomic ions are extremely sensitive to local structure of the ion as well as to dynamical behaviour of molecular species in direct contact with the ion. Theoretical modelling of these parameters can provide molecular-level information typically not accessible by the experimental NMR techniques. The combination of these two methods would thus significantly increase the understanding of mechanisms governing the rate of the quadrupolar relaxation. In this way, simple and abundant monoatomic ions can be used as efficient local probes providing information, for example, about the structure of the active site in a protein or advancing our understanding of correlations between the microstructure of the ionic liquids and their macroscopic properties relevant for rational design of these materials.

Reliable predictions of molecular acidities are of utmost importance because they can assist in a well-motivated selection of most promising drug candidates possessing desired therapeutic values. These molecular parameters determine the protonation state of the molecule which has crucial effect on numerous physiological processes.

Our strength lies primarily in the modelling of spectroscopic NMR and electronic UV/VIS absorption properties of large molecular systems using combined quantum mechanics/molecular mechanics (QM/MM) methods and molecular dynamics simulation techniques. Due to the advanced coupling between the quantum and classical subsystems in the QM/MM model, we are able to realistically model electronic properties of molecular systems composed of tens of thousands of molecules. This opens the door to studying, for example, properties of solvated molecules or protein-ligand complexes of relevance in life sciences. The applications of the molecular dynamics simulations allow studying the dynamical evolution of complex molecular systems and accounting for temperature effects. These yet non-standard computational schemes we have mastered have been successfully used in the areas such as protein-ligand interactions (Fig 1), tautomeric equilibrium in solution or structural and dynamic properties of technologically relevant ionic liquids and their mixtures with water (Fig. 2).

Another area of expertise we possess is quantum chemical modelling of aqueous acidities. The acidity constants are molecular parameters of crucial importance in current state-of-the-art drug development. We have developed computational schemes which have been proven to provide acidities with the accuracy reaching 0.5 pKa unit (Fig. 3). Our computational algorithms are free from adjustable parameters meaning that our methods are universally applicable as opposed to empirical so-called QSPR approaches which typically work well for specific classes of compounds only.

An active line of research is the theoretical characterization of molecular compounds to be potentially used in the areas such as molecular electronics and nanorobotics (Fig. 4). Quantum chemical methods aid in describing relevant structural properties of molecules resulting in favourable excited state structure and charge redistribution processes upon excitation mandatory for the molecular transistors or molecular motors to possess.

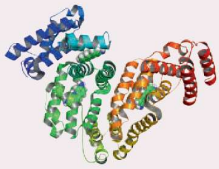

Fig 1. Ligand-bound human serum albumin.

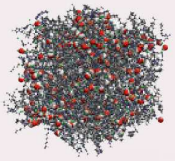

Fig. 2. Ionic liquid mixed with water in the simulation box.

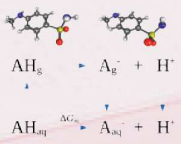

Fig. 3. Towards prediction of the acidity constant.

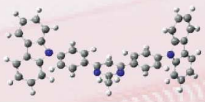

Fig. 4. Potential molecular transistor.

Proposal

We offer our knowledge and experience in designing your spectroscopic measurements and interpreting their results.

We also possess tools to characterize molecular excited states and underlying charge transfer processes as well as to predict acidity constants.

We seek partners for developing competitive research projects targeting HORIZON 2020 and other international programs.

Meet our team

Lead researcher

Dr. **Kęstutis Aidas**

Staff

Assoc. Prof. Dr. **Alytis Gruodis**

Phd students

Dovilė Lengvinaitė

Research outcomes

Most important publications

- **K. Aidas, C. Angeli, K.L. Baketal**. The Dalton quantum chemistry program system. WIREs Comput. Mol. Sci. 4 (2014), 269.
- **K. Aidas, A. Møgelhøj, H. Kjær, C.B. Nielsen, K.V. Mikkelsen, K. Ruud, O. Christiansen, J. Kongsted.** Solvent effects on NMR isotropic shielding constants. A comparison between explicit polarizable discrete and continuum approaches. J. Phys. Chem. A 111 (2007), 4199.
- **K. Aidas, J. Kongsted, A. Osted, K.V. Mikkelsen, O. Christiansen.** Coupled cluster calculation of the n→π* electronic transition of acetone in aqueous solution. J. Phys. Chem. A 109 (2005), 8001.

K. Aidas has obtained postdoc grant of €49000 for the period of 2012-2014 from Lithuanian Science Council. He has been given the Young scientist award by the Lithuanian Academy of Sciences in 2014. K. Aidas is Lithuanian representative in the Management Committee of the COST action CM1405 MOLIM: Molecules in Motion. A grant of €100000 was given to our group by the Lithuanian Science Council to conduct research in the area of theoretical modelling of quadrupolar NMR relaxation, starting from Sept. 1, 2017.

Contacts

Dr. Kęstutis Aidas
Faculty of Physics

Phone: +370 5 223 4593
E-mail: kestutis.aidas@ff.vu.lt

Homepage: web.vu.lt/ff/k.aidas/

Department for Research and Innovation

Phone: +370 5 268 7006
E-mail: innovations@mid.vu.lt

More information: http://www.innovations.vu.lt