PHYSICAL AND TECHNOLOGICAL SCIENCES

Computational Quantum Chemistry Group

Keywords: *Supercomputing, Potential Energy Surfaces, Spectroscopy, Photochromic Properties, Electronic Systems, Carotenoids.*

Vilnius University

Research group activities

In most cases quantum chemical modelling is a necessary component for purposes of characterization of experimental observations. This approach provides the possibility to parametrize smaller molecular parts for further development of other theoretical methods.

On this basis we are analysing ground and excited states of organic electronic systems, such as carotenoids and similar synthetic compounds containing allowed and forbidden electronic states, as well as studying Raman spectra of these systems. Dynamical characteristics of excited states and proton transfer ability by conjugated systems as well as electronic structure of graphene layers are also issues of interest.

Using developed and optimized quantum chemistry codes we are modeling electronic molecular systems relevant to light-harvesting in photosynthetic systems and having applicative potential for molecular electronics.

Since our theoretical modelling is devoted to practical purposes the most of the research carried out in our group is done in tight collaboration with experimental groups. Thus photochromic properties of the light-sensitive molecular systems such as spiropyrans, benzoxazine and carbazole-fluorene-benzothiadiazole compounds, which exhibit changes of absorption properties as a result of photoexcitation, are also the objective of our studies. Due to the specific qualities of these compounds their applicative abilities in molecular-scale electronics and high density data storage seems to be promising.

Resonance Raman spectroscopy, as a vibrational technique, is an ideal method to study structural properties of molecules in their electronic ground state. This approach is also used for studies the environment effect on the spectral properties of conjugated systems by combining resonance Raman and electronic spectra in order to resolve their sensitivity to variability of their surroundings. This experimentally validated modeling technique leads to an explicit understanding of the origin of resonance Raman bands of electronic systems of biological and artificial origin.

Quantum chemical investigations of electronic spectra of structurally deformed carotenoids such as lutein and highly efficient intrinsic phosphorescence from a σ-conjugated poly(silylene) polymer are directly concerned to development of new light-harvesting materials.

Proposal

We offer our knowledge and experience in these research areas:

- Quantum chemical and Molecular Mechanics Modelling;
- Molecular Dynamics Modelling;
- HPC resources up to 25.7 TFlops on 2000 computing cores cluster.

We welcome partners for collaboration in solving the problems of molecular compounds electronic structure.

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

Meet our team

Head - Prof. Dr. Juozas Šulskus

Researchers - Dr. Mindaugas Mačernis, Dr. Stepas Toliautas, Dr. Kazimieras Glemža, Ignas Gaiziūnas, Laurynas Diska, Karolis Jasinevičius

Research outcomes

Selected publications:

- **Karpicz R., Gulbinas V., Lewanowicz A., Mačernis M., Šulskus J., Valkūnas L.** Relaxation pathways of excited N-(triphenylmethyl)salicylidenimine in solutions. J. Phys. Chem. A, 2011, 115 (10), pp 1861–1868.
- **Mačernis M., Šulskus J., Duffy C., Ruban A., Valkūnas L.** Electronic spectra of structurally deformed lutein. J. Phys. Chem. A. 2012, Vol. 116, p. 9843-9853.
- **Duffy C.D.P., Chmeliov J., Mačernis M., Šulskus J., Valkūnas L.**. Modeling of fluorescence quenching by lutein in the plant light- harvesting complex LHCII. . Phys. Chem. B. 2013, Vol. 117, p. 10974-10986.
- **Mačernis M., Šulskus J., Malickaja S., Ruban A.V., Valkūnas L.** Resonance Raman spectra and electronic transitions in carotenoids: a density functional theory study. J. Phys. Chem. A. 2014, Vol. 1178, p. 1817-1825.

Resources

25.7 TFlops supercomputer (2000 computing cores cluster)

Modelling codes: Gaussian, Gamess, Vasp, Crystal, NwChem, Amber, WebMO, Mopac
http://www.supercomputing.ff.vu.lt/?lang=en

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