PHYSICAL AND TECHNOLOGICAL SCIENCES

Dynamical Processes Modelling Group

Keywords: *Excitation and charge transfer, photosynthesis, spectroscopy of molecular complexes, femtochemistry*

Vilnius University

Research group activities

Structure-function relationship in molecular systems of biological and artificial origin is the main objective of studies. Proteins containing chromophoric groups or pigment molecules are known to be sensitive to light conditions. Photosynthetic pigment-protein complexes and reaction centres are well-known examples of such type of systems. Bacteriorhodopsin or rhodopsin - proteins regulating the phototaxis of some bacteria or playing an important role in vision, compose another example of the proteins under consideration. Optical transitions in the chromophoric groups or in pigment molecules play a role of a trigger of the activity of these proteins. Together with biological complexes the systems of artificial and non-biological origin, such as hybrid perovskites, carbon nanotubes etc., which are of interest of their applicative potential, are also investigated by the research group in tight collaboration with various experimental groups.

Our group is interested in modelling various dynamical processes in complex condensed phases and molecular systems. We are currently investigating energy transfer and charge separation in natural and artificial photosynthetic systems, as well as in nanomaterials of technological interest. We are studying photoprotection, damage, and adaptation mechanisms of biological systems, especially in photosynthetic organisms. All these studies are carried out in tight collaboration with experimental groups and with groups of Computational Quantum Chemistry and Physics of Open Quantum Systems from Faculty of Physics at Vilnius University.

Proposal

Models developed by the group are based on quantum chemical description of the systems under consideration and on the quantum mechanical characterization of excitation and charge evolution as a result of perturbation of the electronic degrees of freedom. All these models are approved by analysing various experimental data, thus, demonstrating ability to resolve the structure-function relationship of the systems under consideration.

A special attention is paid for understanding the influence of the environment (or proteins and their environment in the biological systems) on the photoinduced dynamical processes. This problem has also a direct applicative aspect by searching for novel approaches suitable for molecular electronics or nanobiotechnology as well as for optimisation possibilities in photovoltaics.

We are searching for partnership in HORIZON 2020.

Meet our team

Leader of the group - **Prof. Habil Dr. Leonas Valkūnas**

Other team members - Assoc. Prof. Dr. **Jevgenij Chmeliov**, Dr. **Vytautas Butkus**, Dr. **Andrius Gelžinis**, Prof. Habil. Dr. **Vytautas Balevičius** Jr., Assoc. Prof. Dr. **Juozas Bučinskas**

Research outcomes

Scientific results obtained by members of the group are published in 55 scientific publications in such journals as Nature Chemistry, Nature Communication, Nature Plants, J. Phys. Chem. Lett., J. Phys. Chem., Phys. Chem. Chem. Phys., Nanoscale, etc.; one book: L. Valkunas, D. Abramavicius, T. Mancal. Molecular excitation dynamics and relaxation. Quantum theory and spectroscopy. Wiley-VCH, Weinheim, 2013; and four chapters in the scientific books during the last 5 years.

Resources

High performance computing open access center “HPC-Saulėtekis” with 2000 computing cores cluster.

Contacts

Prof. Habil. Dr. Leonas Valkūnas
Faculty of Physics

Phone: +370 5 2366030, +370 5 2234662
E-mail: leonas.valkunas@ff.vu.lt

Home page: http://web.vu.lt/ff/l.valkunas/

Department for Research and Innovation

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

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