PHYSICAL AND TECHNOLOGICAL SCIENCES

# Physics of Open Quantum Systems

Vilnius University

***Keywords:*** *relaxation dynamics, non-equilibrium processes, excitons, polarons, dissipatons, energy transport, charge transport, nonlinear spectroscopy, coherent dynamics*

## Research group activities

Atomic crystalline semiconductors are widely used in electronic circuits and photovoltaics. However, the material properties put restrictions on operating speeds and/or on quantum yields and efficiencies. There is a constantly growing interest in alternative materials, which are amorphous, polycrystalline or molecular-based. Organic electronic is very promising in photovoltaic and in light sources. Specific photoactive molecular materials are also involved in skin protection design as well as drug and nutrition development. Functioning basis in this kind of materials relies upon photo-induced relaxation dynamics. Quantum relaxation theory of the open quantum systems describes the process. Experimentally such systems are usually studied by laser spectroscopy that can be described by using the response function theory. Description of such systems using the response functions of open quantum systems is the main subject of the research of the group.

The main objects of our studies are typical model systems (spin-boson model, excitonic molecular aggregates described by Holstein model, multilevel quantum systems), photosynthetic molecular aggregates, and molecular-based photovoltaic prototypes. Some of them are used in developing molecular devices. Internal non-equilibrium processes in such objects are still obscure, especially immediately after photoexcitation. Developing theoretical approached to describe physical phenomena may shed light on mechanisms of functioning and may lead to improvements in molecular designs for specific devices.

## Proposal

- We offer numerical computing expertize, as we write computer programs and perform scientific computing. We have our own computer codes to calculate coherent two-dimensional spectroscopy signals for excitonic systems coupled to continuous spectral density environment at a constant temperature.
- We seek partners for developing competitive research projects targeting HORIZON 2020 and other international programs.

## Meet our team

Leader of the group - Prof. Dr. **Darius Abramavičius**

Senior research member - Dr. **Olga Rancova**

Undergraduate researchers - **Mantas Jakučionis, Vytautas Bubilaitis**

PhD students are welcome to join.

We have close collaboration with Quantum Chemistry and Molecular dynamics group in Vilnius University as well as with international partners at Queen Mary University in London UK, University of Vienna Austria, Kansas State University and University of Michigan in USA, University of Copenhagen Denmark.

## Research outcomes

### Selected publications

We earned a high level of citation record and won several national scientific grants and awards.

- **V. Butkus, L. Valkunas, D. Abramavicius**, Vibronic phenomena and exciton–vibrational interference in two-dimensional spectra of molecular aggregates, J. Chem. Phys. 140, 034306 (2014).
- **O. Rancova, R. Jankowiak, D. Abramavicius**, Probing environment fluctuations by two-dimensional electronic spectroscopy of molecular systems at temperatures below 5 K, J. Chem. Phys. 142 , 212428 (2015).
- **D. Abramavicius, L. Valkunas,** Artificial Photosynthesis: Theoretical Background. In R. Bruno (Ed.), Artificial Photosynthesis, pp. 129–167 (2016).
- **V. Chorošajev, O. Rancova, D. Abramavicius**, Polaronic effects at finite temperatures in the B850 ring of the LH2 complex, Phys. Chem. Chem. Phys., 18, 7966 (2016).
- **V. Abramavicius, V. Pranculis, A. Melianas, O. Inganäs, V. Gulbinas, D. Abramavicius,** Role of coherence and delocalization in photo-induced electron transfer at organic interfaces, Sci Rep. 86, 32914 (2016).

## Resources

- A computer cluster of 24 nodes for development of computer codes.
- Supercomputer “Altix UV 1000” (120 Intel x86_64 Cores, 2.5 TB RAM, Rmax:1.160e+03 Gflops).

## Contacts

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