

The Warsaw Doctoral School in Natural and Biomedical Sciences and the Institute of Physics PAS cordially invites you to a **SPOTLIGHT TALK**

Light-induced Reactions in Cryogenic Matrices

given by

Dr. Igor Reva

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on 17th September 2024, 10:30 at the IP PAS Leonard Sosnowski Auditorium

Duration: 45 min + question time

The event will be available on ZOOM also, at this link

All Warsaw-4-Phd students (and others) very welcome!

Abstract of the talk:

Studies on the photochemical reactivity and characterization of the primary photoproducts permit a deeper understanding of reaction mechanisms. In this talk, the experimental technique of low temperature matrix isolation allowing to experimentally test the incipient steps of photochemical reactions, and to characterize novel species with unusual functionalities, properties and behavior will be addressed.

We shall start with the fundamentals of the method and show its possibilities in the studies of structure and reactivity at cryogenic temperatures (~10 K). Typically, the molecules are embedded in solid inert matrices (Ar, Xe, N₂) and excited *in situ* either by a broadband light source, such as Hg/Xe lamp, or by narrowband light generated in an optical parametric oscillator or in a diode laser. The structures of reactants and photoproducts are characterized experimentally by infrared spectroscopy and theoretically by computation of vibrational spectra.

The potential of the method will be demonstrated using several conformational studies. Narrowband near-infrared irradiations, tuned at the frequencies of the OH or NH first overtone modes, result in conformational switching. Hereby, it becomes possible to characterize high-energy conformers, not accessible experimentally otherwise, and study processes of intramolecular vibrational energy transfer. The examples will include carboxylic acids, amino acids, nucleobase cytosine, among others. Besides, the isomerizations occurring in matrix-isolated molecules in dark (H-atom and heavy-atom tunneling) and those induced by the light source of the spectrometer will be discussed.

Further examples concern the reactivity induced by frequency-tunable UV light. Here, H-atom transfer reactions, resulting in oxo-hydroxy, amine-imino, thiol-thione isomerism, for phenol, cytosines, thiophenol, and some heterocycles will be described.

In general, this contribution will provide a selection of experimental and computational results, co-authored by the presenter [1], providing insight into the observed reactivity.

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Igor Reva graduated in Biophysics, with honors, from the Kharkiv State University. Upon graduation, worked for several years as engineer, at the Institute for Low Temperature Physics & Engineering (ILTPE), a major research centre of the National Academy of Sciences of Ukraine (in Kharkiv), where he mastered diverse technical aspects of cryogenic applications.

In 1995, completed a PhD degree in Molecular Physics & Biophysics, at ILTPE.

In July 1997 – September 1999, Igor Reva was awarded a post-doctoral fellowship of the Alexander von Humboldt Foundation at Max-Planck-Institute (MPI) for Radiation Chemistry (Mülheim-an-der-Ruhr, Germany) and MPI for Nuclear Physics (Heidelberg, Germany).

Since October 1999 and until 2020, moved to the University of Coimbra (UC), Portugal, where he worked as: (i) post-doctoral fellow of the Portuguese “Fundação para a Ciência e a Tecnologia” (FCT), (ii) Researcher (FCT program “Science-2007”), (iii) Principal Researcher (program “Investigador FCT”), all above positions at the Centre of Chemistry of Coimbra, Department of Chemistry (DQ) at UC. Since 2021 (till present), Igor Reva works at the Research Centre hosted at the Department of Chemical Engineering (DEQ) at UC. Since 2024, this research centre at DEQ/UC is named CERES (from Portuguese: “Chemical Engineering and Renewable Resources for Sustainability”).

In 2010, the degree of Habilitation in Chemistry was conferred on Igor Reva by UC, with specialization in Molecular Spectroscopy.

The engineering skills and qualification, acquired by Igor Reva at ILTPE, allowed him subsequently to design and construct in Portugal (at DQ/UC) a home-made fully operational experimental setup for matrix-isolation spectroscopy and photochemistry at cryogenic temperatures. This setup is now an integrated part of Coimbra Laser Lab (CLL), hosted at DQ/UC. CLL is a Research Infrastructure of FCT established at UC and is a part of LaserLab Europe - Consortium of European Laser Research Infrastructures (35 organizations from 18 countries). At CLL, Igor Reva provided scientific supervision and technical training for users from +20 countries.

Main specializations of Igor Reva are infrared spectroscopy, photochemistry, photochromic molecules, molecular switches, reactive intermediates, systems with open electronic shells, quantum mechanical tunneling, including their experimental and computational studies.

He participated in +30 competitively funded FCT projects (in 8 as principal investigator). As of September 2024, published +170 articles in peer-reviewed journals, in 1/3 of these Igor Reva is the corresponding author. H-index: 42 (Publons) / 43 (Scopus), with +5 K citations.

Considering the present STER application to NAWA, it should be noted that Igor Reva participated in two bilateral projects with IF PAN, acting as coordinator for the Portuguese side. Each of these two projects lasted two years. Collaborations with researchers from IF PAN resulted in 42 joint peer-reviewed publications.

[1] A detailed research CV of Igor Reva can be found at the following URL: <http://www.cienciavita.pt/en/C810-38EA-F1A6>

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