

3rd International Conference and Exhibition on Materials Science & Engineering

October 06-08, 2014 Hilton San Antonio Airport, USA

Photoexcited conjugated chromophores: Conformational dynamics, relaxation pathways and energy transfer

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Prediction and understanding of photoinduced processes in molecular- and nano-materials is fundamental to a myriad of technological applications, ranging from sensing, imaging, solar energy harvesting, to future optoelectronic devices. Thereby modelling of non-adiabatic dynamics in extended molecular systems and solids is a next frontier of atomistic electronic structure theory. Using our recently developed non-adiabatic excited-state dynamics simulations framework, we study ultrafast dynamics and exciton transport in several large molecular systems. These simulations reveal a fascinating interplay of conformational vibrational dynamics and internal conversion followed photoexcitation, which has specific spectroscopic signatures and can be observed using time-resolved pump-probe spectroscopies. Observed relationships between spatial extent/properties of electronic wavefunctions and resulting electronic functionalities allow us to understand and to potentially manipulate excited state dynamics and energy transfer pathways in a number of organic molecular materials suitable for a variety of technological applications.

Biography

Sergei Tretiak received his MSc degree (highest honors, 1994) from Moscow Institute of Physics and Technology (Russia) and his PhD degree in 1998 from the University of Rochester where he worked with Prof. Shaul Mukamel. Afterwards he was Director-funded Postdoctoral Fellow (1999-2001) and subsequently became a Technical Staff Member at LANL (2001-present). Since 2006 Tretiak is a member of the DOE funded Center for Integrated Nanotechnologies (CINT). He is also serving as a Founding Faculty Fellow at Skolkovo Institute of Science and Technology, Moscow, Russia (2013-present). He received the LANL 2010 Fellow's Prize for Research. His research interests include development of modern computational methods for molecular optical properties, nonlinear optical response of organic chromophores, adiabatic and non-adiabatic molecular dynamics of the excited states, optical response of confined excitons in conjugated polymers, carbon nanotubes, semiconductor nanoparticles, and molecular aggregates. He has published over 170 scientific publications cited over 6000 times and has presented more than 150 invited talks in the US and abroad.

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