DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
SEMINAR SERIES
SPRING 2022

DATE: WEDNESDAY, MAY 4

WEBEX:
https://njit.webex.com/njit/j.php?MTID=ma36c0efbccd3176c875d112fbc50a7e4
Meeting number: 2621 165 2481
Meeting password: NmbmssWm325

TIME: 1:00PM-2:20PM

GUEST SPEAKER

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TOPIC

Multiscale modeling of molecular systems and materials: the case of energy transfer

ABSTRACT

I will introduce the advantage of multi-scale modeling strategies and present some examples where we have successfully applied them to model different kinds of properties and processes in molecular materials. I will then focus on presenting an application to Resonance Energy Transfer (RET). In this process, the energy is transferred from an excited molecule, called the energy donor (D), to an acceptor molecule (A). We have investigated Förster RET for a pair of dyes linked to a calixarene scaffold. In such systems, the relative orientation of the D and A changes on a time-scale comparable to RET dynamics, making the two limiting regimes, static and dynamic, hardly applicable. In the advanced multiscale approach to the dynamics of RET, we combine DFT and TD-DFT results on the energy donor (*D*) and acceptor (*A*) moieties with an extensive equilibrium and non-equilibrium molecular dynamics (MD) analysis of a bound *D–A* pair in solution to build a coarse-grained kinetic model. We demonstrate that a thorough MD study is needed to properly address RET: the enormous configuration space visited by the system cannot be reliably sampled accounting only for a few representative configurations. Moreover, the conformational motion of the RET pair, occurring in a similar time scale as the RET process itself, leads to a sizable increase in the overall process efficiency. This work solved a major issue related to the characterization of RET rates in systems with high flexibility, emphasizing the importance of a dynamical approach for the description of complex decay mechanisms and opening up new opportunities for their theoretical treatment.

BIO

After the Master's Degree in Chemistry at Parma University (Italy), with a Physical Chemistry curriculum, in 2011 received his Ph.D. in Chemical Sciences in the same university as both

experimentalist and theoretician working on a thesis project "Charge and energy transfer in functional molecular materials: spectroscopy and models". From 2011 to 2013 he was Post-doc at the University of Mons (Belgium) in the "Chemistry of Novel Material" group of prof. D Beljonne and J. Cornil, working mainly in the field of organic molecular electronics (development of computational approaches for charge and exciton transport in molecular materials). From 2013 to 2016 Luca was a Post-doc at the "International Centre for Theoretical Physics" (ICTP) in Trieste, (Italy) working in computational material science and biophysics, including modeling of biomaterial and biomolecule from morphology to electronic structure and optical properties. From 2016 to 2018 he joined SISSA (Trieste, Italy) as a Post-doc, working on modeling and computation of optical properties of bio-molecules. In 2018 he became an associate researcher at the Division of Theoretical Physics of the Institut Ruđer Bošković (Zagreb, Croatia), working in the group on material modeling and he's involved in several research projects. Beyond academics, he is interested in science communication and dissemination.

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