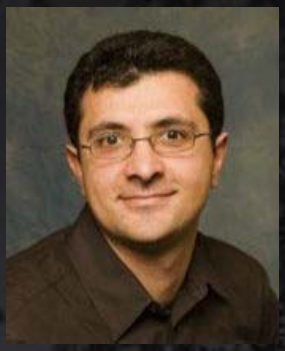
CENTER FOR EXCITONICS SEMINAR SERIES

Less is more: model reduction for exciton and charge transport in molecular materials



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We present a common strategy to address questions concerning the charge and energy transfer in organic molecular materials and aggregates. This is based on the construction of reduced (predictive) models from (detailed) atomistic one. We will argue that, somewhat counterintuitively, by removing chemical detail from the model one can more easily perform chemical predictions or derive chemical rules. The topic considered in this lecture include (i) the definition of a map of all organic semiconductors for charge transport; (ii) the desirable properties of electron acceptors in organic solar cells; (iii) the degree of structural fine tuning that can be observed in natural light harvesting complexes.

Alessandro Troisi received his PhD in Physical Chemistry in 2001 from the University of Bologna for his research on the charge transfer reactions in condensed phases. As a postdoctoral researcher at Northwestern University in Mark Ratner's group, he worked on single molecule electronics. During this time, he also studied electron transport through flexible molecules and developed a model for inelastic tunneling spectroscopy. In 2004-2005, he was a research fellow at the University of Bologna studying the charge transport mechanism in organic solid crystals. In October 2005, he joined the Department of Chemistry at the University of Warwick as a Research Council UK Fellow and in 2010 as a Professor until 2017. Currently, he is a Professor of Chemistry at the University of Liverpool. He has received numerous awards including the Marlow Award of the Royal Society of Chemistry, the ERC - Starting Investigator Award (2009) and the ERC - Consolidator Grant (2013).

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