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The Splendors and Miseries of Exciton Models

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ABSTRACT

Exciton models offer an opportunity to simulate the optoelectronic properties of large disordered molecular systems that cannot be adequately described either by ab initio quantum chemical methods or by band theory. Such systems include organic photovoltaic blends, natural and artificial photosynthetic complexes, and organic electro-optic materials. Exciton models are useful for studying a variety of processes including linear and nonlinear optical response, energy transfer, and charge separation. However, the computational efficiency of these models is a direct consequence of approximations that underlie their construction.

In this talk I will assess the accuracy of exciton models for calculating the absorption spectra of large chromophore aggregates, benchmarked against large-scale TDDFT calculations. I will show that accounting for the local molecular environment in the parametrization of exciton models is critical to their performance. I will also explore how these models can be used in computational studies of nonlinear refraction in electro-optic materials. Finally, I will demonstrate the convenience of exciton models for simulations of ultrafast charge separation in donor-acceptor dyads and present insights into the role of high-energy charge transfer states gained from these simulations.

BIO:

Aleksey Kocherzhenko received a PhD in physical chemistry from Delft University of Technology, where he worked as a Marie Curie fellow in the Optoelectronic Materials Section under the guidance of Dr. Ferdinand Grozema and Dr. Laurens Siebbeles. He then spent three years as a Rubicon fellow in the group of Dr. Birgitta Whaley at the Pitzer Center for Theoretical Chemistry, UC Berkeley. He is currently a postdoc in the group of Dr. Christine Isborn at the Department of Chemistry and Chemical Biology, UC Merced. His recent work has focused on the development of computationally efficient techniques for modeling optical and electronic processes in disordered organic materials.