

VISTA Seminar

Seminar 44

November 2, 2022

**10:00 am – 11:30 am EDT / 2:00 – 3:30 pm GMT London / 3:00 pm –
4:30 pm CET Paris / 10 pm CST Beijing**

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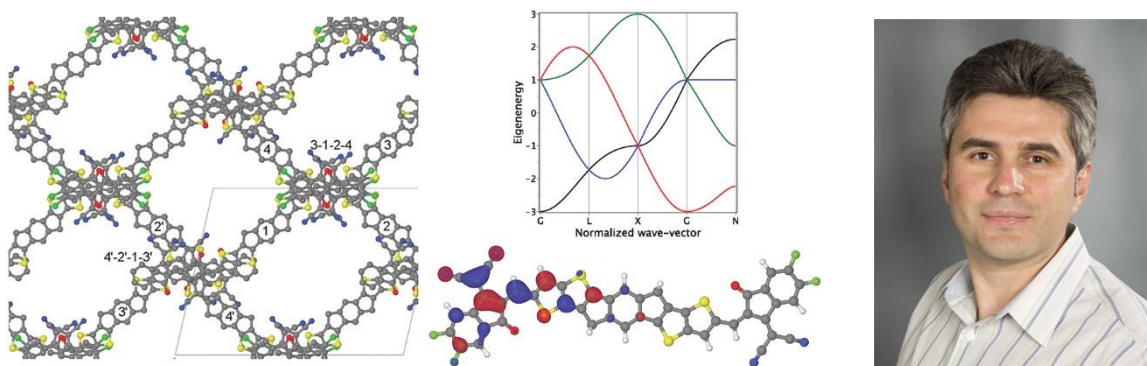
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Nonadiabatic dynamics at large scales from perspective of applications to organic semiconductors

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Electron-phonon interaction in semiconductors is always important for the understanding of their optoelectronic properties such as charge carrier mobility because their frontier orbitals are typically composed of bonding and antibonding orbitals. In many materials, this interaction can be considered perturbatively, but whenever electronic and vibronic couplings are comparable in magnitude, the electron-phonon dynamics becomes complicated. In such cases, we usually understand the mechanisms of electron-phonon interactions, have tools for accurate modeling of nonadiabatic dynamics at small scales, and can resort to simplified lattice models to grab the essence of large-scale phenomena. At the same time, first-principles modeling of real-world materials remains challenging because known scalable methods contain a lot of uncontrolled approximations, whereas a very limited amount of reference data for methodology validation is available, either experimental or of higher-level theory. This is the case for organic semiconductors, and in the first part of my talk I will discuss open questions in the modeling of these materials (related to nonadiabatic dynamics) for various applications such as solar cells [1] and metal-ion batteries [2]. Then in the second part I will focus on a particular problem: how to reduce the basis of the electronic part of the Hamiltonian and how to parameterize the latter from DFT calculations. This can be called electronic coarse-graining: constructing a minimal basis that provides an accurate description of frontier orbitals and near-gap excitations under thermal fluctuations. For small-molecule solids, the solution is trivial – one electronic state per molecule, but a general case requires a more elaborated approach, examples include long oligomers [1] and polymers [2].

References

[1] S Halaby, M W Martynowycz, Z Zhu, S Tretiak, A Zhugayevych, T Gonen, M Seifrid, Microcrystal Electron Diffraction for Molecular Design of Functional Non-Fullerene Acceptor Structures, *Chem Mater* 33, 966 (2021)

[2] R Kapaev, A Zhugayevych, S Ryazantsev, D Aksyonov, D Novichkov, P Matveev, K Stevenson, Charge storage mechanisms of a pi-d conjugated polymer for advanced alkali-ion battery anodes, *Chem Sci* 13, 8161 (2022)

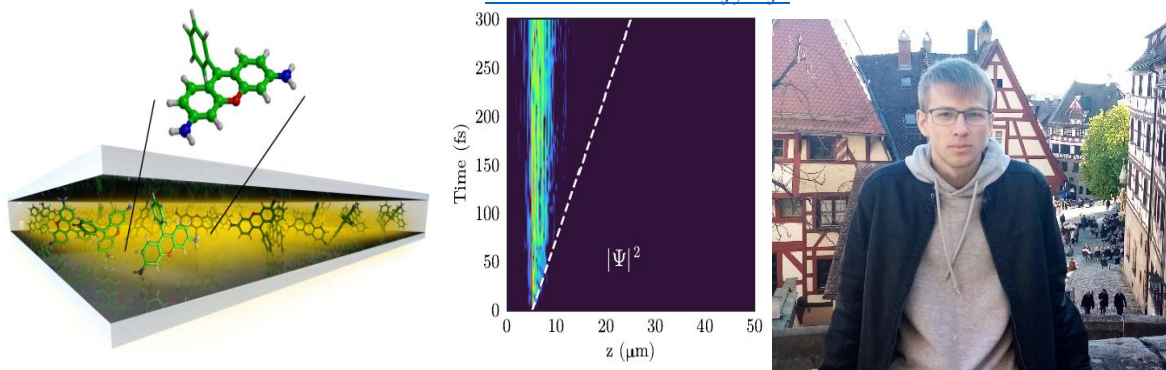
Enhanced Energy Transport under Strong Light-Matter Coupling: Insights from Molecular Dynamics Simulations

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Transfer of excitation energy is a key step in light harvesting and hence of huge technological relevance for solar energy conversion. In bare organic materials, energy transfer proceeds via incoherent hops, which restrict propagation lengths to the nanoscale[1]. This imposes a limitation on the thickness of the active layer of organic solar cells and, as a consequence, on their efficiency. In contrast, energy transport over several micrometers has been observed in the strong coupling regime where excitations hybridize with confined light modes to form polaritons[2-7]. Because polaritons inherit the group velocity of the confined light modes, their propagation is ballistic and long-ranged. However, experiments on organic microcavities indicate that polaritons propagate in a diffusive manner and much more slowly than the polariton group velocity. In this study, we resolve this controversy by means of atomistic multiscale molecular dynamics simulations of Rhodamine molecules in a Fabry-Perot cavity. Our results suggest that polariton propagation is limited by the cavity lifetime and appears diffusive due to reversible population transfer between bright polaritonic states that propagate ballistically at their group velocities, and dark states that are stationary. Furthermore, because the long-lived dark states can effectively trap the excitation, propagation is observed on timescales far beyond the intrinsic polariton lifetime. The atomistic insights from our simulations not only help to better understand and interpret experimental observations, but also pave the way towards rational design of molecule-cavity systems for achieving coherent long-range energy transport.

References

- [1] O. V. Mikhnenko, P. W. M. Blom, T.-Q. Nguyen, *Energy Environ. Sci.*, 8, 1867-1888, 2015
- [2] D. Ballarini et. al., *Light Sci. Appl.*, 6, e16212, 2017
- [3] G. G. Rozenman, K. Akulov, A. Golombek, and T. Schwartz, *ACS Photonics*, 5, 1, 105-110, 2018
- [4] S. R. Forrest et. al., *Adv. Mater.*, 32, 28, 2002127, 2020
- [5] R. Pandya et. al., *Nat. Commun.*, 12, 6519, 2022
- [6] R. Pandya et. al., *Adv. Sci.*, 2105569, 2022
- [7] A. M. Berghuis et. al., *ACS Photonics*, 9, 7, 2263-2272, 2022

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Topic: VISTA, Seminar 44

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