Department of Chemistry
Faculty of Exact Sciences
Bar-Ilan University

The Department of Chemistry Weekly Seminar Wednesday 11/5/22 at 11:00am (Refreshments 10:45am)

Quantum Transport in Organic Semiconductors

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In the first part of the talk, I will present calculations of coherent charge and exciton transport in disordered organic systems, which reveal an optimal diffusion constant at the crossover between the coherent and incoherent regimes.[1] The quantum enhancement in the coherent regime depends on the dimension and shape of the sample and exhibits a universal scaling.[2] Mapping of quantum to kinetic networks provide both an intuitive understanding of these coherent features and a potentially useful numerical technique. Though transport is suppressed by disorder, trapping or dissociation can be enhanced by disorder.[3]

In the second part of the talk, I will discuss recent results on quantum diffusion assisted by phonons or cavity photons. Our analysis of the tilted Holstein model predicts the fractional vibronic resonance, which is supported by mapping the Holstein model to a continuous time random walk.[4] In optical cavities, disordered organic molecules are coupled to cavity fields collectively, such that the cooperativity in the light-matter interaction can overcome the Anderson disorder and lead to a turnover in transport at an optimal level of static disorder.[5]

1. Coherent quantum transport in disordered systems: I. The influence of dephasing on the transport properties and absorption spectra on one-dimensional systems. Moix, Khasin, Cao, New Journal of Physics, 15, 085010 (2013)
2. Quantum diffusion on molecular tubes: Universal scaling of the 1D to 2D transition. Chuang, Lee, Moix, Knoester, and Cao, Phys. Rev. Lett. 116, 196803 (2016)
3. Generic mechanism of optimal energy transfer efficiency: A scaling theory of the mean first-passage time in exciton systems. Wu, Silbey, Cao, Phys. Rev. Lett 110 (20), 200402 (2013)
4. Long-range non-equilibrium coherent tunneling induced by fractional vibronic resonances. Kessing, Yang, Manmana, Cao, arXiv:2111.06137 (2021)
5. Unusual dynamical properties of disordered polaritons in microcavities. Engelhardt and Cao PRB 105(6), 064205 (2022)

Location: Seminar Room 112

Looking forward to seeing you!