VISTA Seminar

Seminar 49

April 12, 2023

10:00 am – 11:30 am EST / 3:00 – 4:30 pm GMT London / 4:00 pm – 5:30 pm CET Paris / 11 pm CST Beijing

TOC:

Non-equilibrium electron dynamics from real-time quantum embedding

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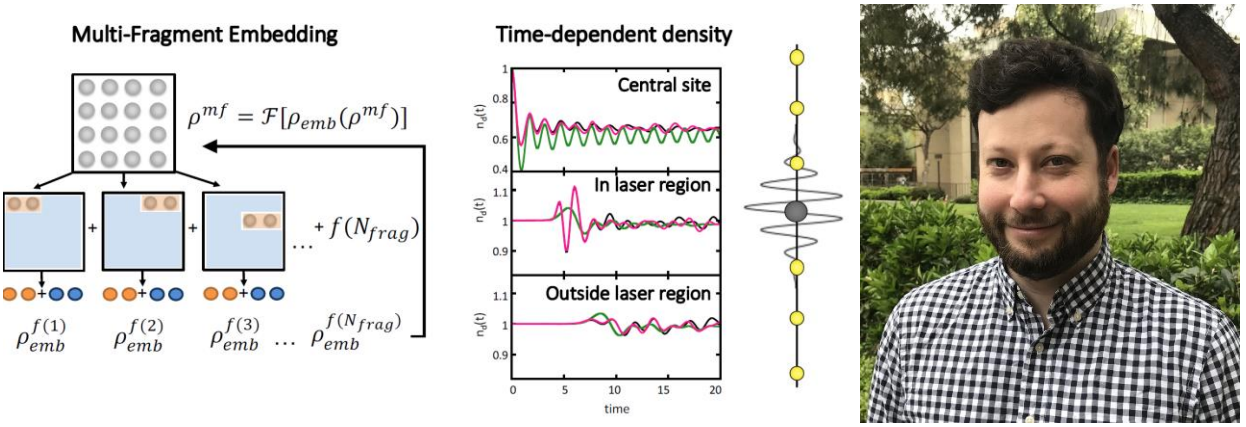

Spin-selective transport through materials and molecules involves unique and subtle effects not normally associated with charge transport. To unravel such complex physics, it is necessary to develop new simulation methods that allow for the unbiased investigation of the non-equilibrium electron dynamics underpinning these systems. Towards this goal, we present our work on the development of a real-time formulation of the projected density matrix embedding theory (pDMET). In real-time pDMET, the total system is partitioned into multiple fragments, each coupled to an effective quantum bath representing the interaction with the surrounding environment. Each of these separate embedding problems are propagated in time along with an auxiliary mean-field wavefunction of the total system. The methodology allows for the efficient and accurate simulation of non-equilibrium electron dynamics in the presence of strong correlation, reaching total system sizes unobtainable by conventional methodology.

Simulating the photophysics of DMABN: what have we learned, and where do we go from here?

Michał Andrzej Kochman

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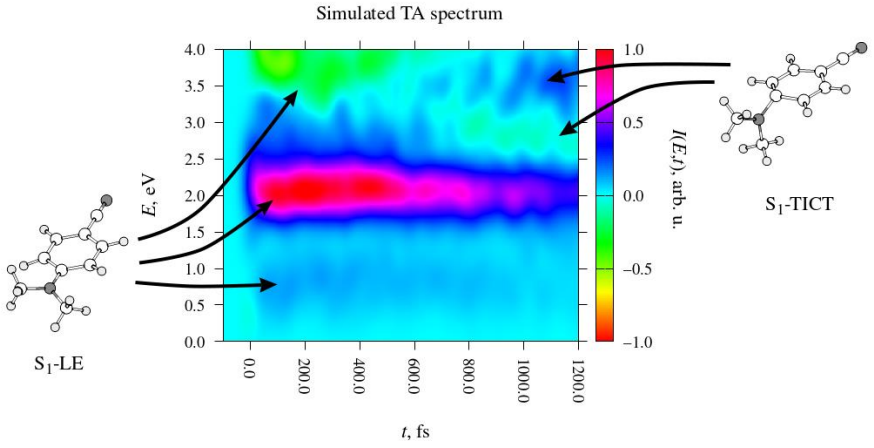

4-(*N*,*N*-dimethylamino)-benzonitrile (DMABN) is a model compound for dual fluorescence – in solvents of sufficiently high polarity, it exhibits two distinct fluorescence bands, of which one (the so-called "normal" band) has a small Stokes shift, and the "anomalous" second band is strongly red-shifted. Many aspects of its photophysics, and especially the structure of the species which is responsible for the anomalous band, have been the subject of long-standing controversy.

In this talk, I will outline my efforts to clarify the dual fluorescence mechanism of DMABN with the use of computer simulations. In particular, I will examine the relationship between the topography of the S_2–S_1 conical intersection seam and the sequence of events following photoexcitation to the S_2 state. I will show how the calculation of time-resolved fluorescence and transient absorption (TA) spectra provides a direct connection between simulation results and spectroscopic data. Lastly, I will discuss the implications of this research for the study of larger donor-acceptor compounds with applications in organic optoelectronics.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 49
Time: Apr 12, 2023 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting
https://buffalo.zoom.us/j/93558101236?pwd=b21sZmlGdkJTbGNxSFg2WlZEWitsZz09

Meeting ID: 935 5810 1236
Passcode: 384181