VISTA Seminar

Seminar 19

May 26, 2021

9:30 – 11:00 am EDT / 1:30 – 3:00 pm GMT / 3:30 pm – 5:00 pm Paris

TOC:

Exciton many-body dynamics in organic and hybrid 2D semiconductors.

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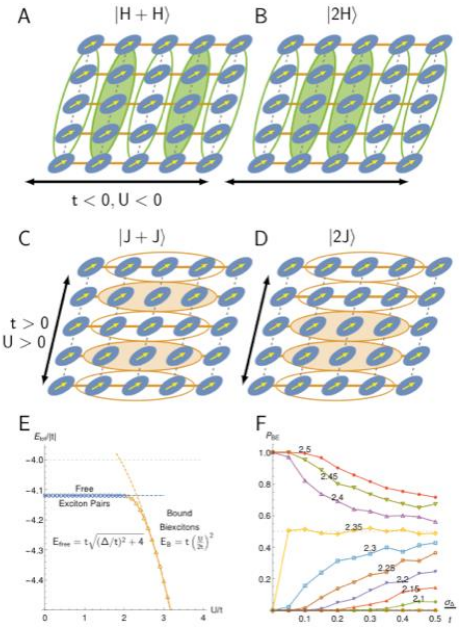

Exciton/exciton interactions account for a wide range of photo physical processes in semiconducting materials. In my talk, I will present highlights of our recent theoretical work which seeks to unravel the signatures of exciton many-body dynamics as revealed in 2D coherent spectroscopic signals. I will first discuss our quantum stochastic model for excitation-induced dephasing in which we treat background excitations as a non-stationary mean-field which co-evolves with the optical signal. The model reduces to the well-known Anderson/Kubo form at long times and reveals how transient non-stationary effects impact both linear and non-linear spectral signals.

The second part of my talk will focus upon the formation of stable biexcitons in H and J-like conjugated polymer systems. Generally, bound states arise due to attractive interactions between pairs of particles. Surprisingly, we find evidence for bound biexciton states arising from repulsive and attractive exciton/exciton interactions. Using basic quantum mechanics and rigorous many-body theory, we show how such seeming contradictory states can occur and present a theoretical phase diagram correlating specific material parameters such as exciton band-width, inhomogeneous disorder, variation in local energetics, and exciton/exciton interaction strength to the stability of the biexciton state.

Machine Learning for Surface Hopping Molecular Dynamics: The Case of Excited Tyrosine

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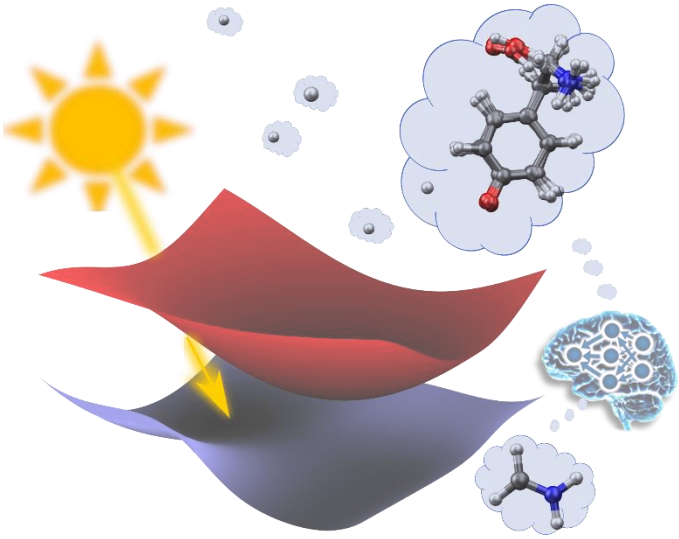

Machine learning (ML) methods are powerful tools to support nonadiabatic molecular dynamics simulations by decoupling the costs of the underlying electronic structure calculations from the dynamics simulations. However, the bottlenecks of finding and applying accurate *ab initio* excited state methods for complex molecular systems also limit the use of ML models. Consequently, only a few studies go beyond model systems or a few excited states [1]. In this talk, we will introduce the SchNarc approach [2] for photodynamics simulations and demonstrate the accuracy of this approach on the example of the methylenimmonium cation [2,3]. Additional challenges arise for studying the excited states of tyrosine, which will be discussed and require that the ML model incorporates underlying physics of the data. Our novel ML potentials enable photodynamics simulations of highly excited tyrosine that can complement experimental findings. Further, the simulations suggest an unexpected reaction mechanism and provide new insights into the photochemistry of biological matter [4].

References:

[1] J. Westermayr, P. Marquetand *Chem. Rev.*, in press, doi:10.1021/acs.chemrev.0c00749 (2020).
[2] J. Westermayr, M. Gastegger, P. Marquetand *J. Phys. Chem. Lett.* **11**(10), 3828-3834 (2020).
[3] J. Westermayr, M. Gastegger, M. Menger, S. Mai, L. González, P. Marquetand *Chem. Sci.* **10**, 8100-8107 (2019).
[4] J. Westermayr, *et al.* unpublished (2021).

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 19
Time: May 26, 2021 09:30 AM Eastern Time (US and Canada)

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