

VISTA Seminar

Seminar 38

May 25, 2022

10:00 am – 11:30 am EDT / 3:00 – 4:30 BST / 4:00 pm – 5:30 pm Paris

TOC:

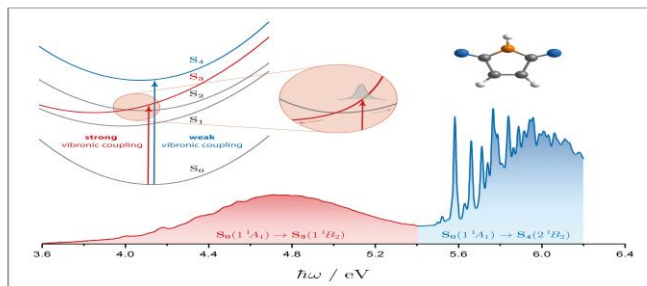
1. Presenter 1: Prof. Graham Worth, University College London, UK..... page 2
2. Presenter 2: Dr. Thierry Tran, University College London, UK..... page 3
3. How to connect..... page 4

From Grids to Gaussians. Non-adiabatic Simulations with the Quantics Package

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Over the last couple of decades a number of different approaches to simulate the dynamics of photo-excited systems involving non-adiabatic coupling between electronic states. These range from accurate grid-based solutions to the time-dependent Schrödinger equation (TDSE) to simple trajectory based methods simulating the time evolution of the evolving wavepacket.

In this talk I will give an overview of the multi-configurational time-dependent Hartree (MCTDH) family of methods [1]. In the grid-based form of ML-MCTDH [2], these can accurately treat systems with many (over a hundred) degrees of freedom, but require simple Hamiltonians such as the linear vibronic coupling model [3]. In the Gaussian wavepacket-based form of G-MCTDH [4], we can use more realistic, flexible potentials, and in the form of DD-vMCG can even calculate the potential surfaces on the fly [5]. Examples will be used to show the abilities of the methods.

All of these methods (and more) have been implemented in the Quantics Package [6].

References

- [1] M. Beck et al, Phys. Rep., 324:1, 2000.
- [2] Vendrell and Meyer, J. Chem. Phys., 134: 44135, 2011.
- [3] G. A. Worth et al. Int. Rev. Phys. Chem., 27:569, 2008.
- [4] G. W. Richings et al. Int. Rev. Phys. Chem., 34:269, 2015.
- [5] J. Coonjobeechary et al Phil. Trans. Roy. Soc. A, 380:20200386, 2022.
- [6] G. A. Worth. Comp. Phys. Comm., 248:107040, 2020.

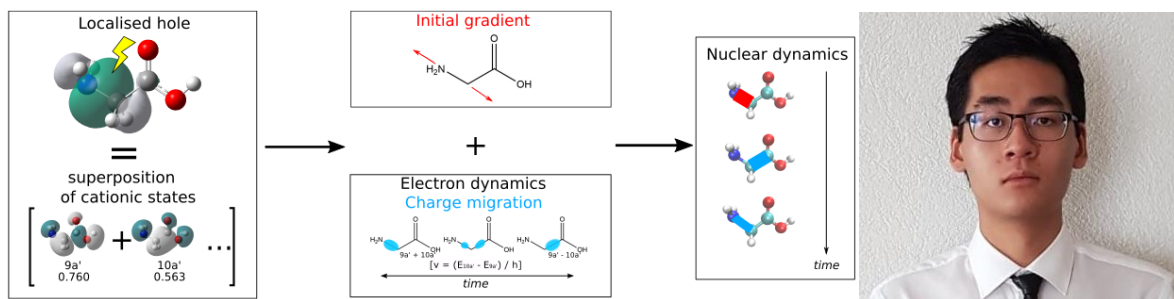
Simulation of fast electron dynamics using an Ehrenfest approach with DD-vMCG (QuEh): Application to charge migration driven nuclear dynamics

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The coupled electron-nuclear dynamics of molecular system is described using a fully quantum approach. Starting from the exact factorization ansatz [1], the Quantum-Ehrenfest method [2] is obtained by expanding the nuclear wavefunction as a sum of gaussians following ‘quantum’ trajectories [3] on an Ehrenfest potential energy surface. This approach allows us to initiate the simulation with an arbitrary electronic wavefunction such as a coherent superposition of states.

The method was employed to simulate the charge-directed dynamics of retinal protonated Schiff base [4], benzene [5] and ethylene cations upon photoionization with an ultrashort pulse in the UV to XUV region. The resulting dynamics and initial nuclear gradient are heavily controlled by electronic coherence and can be rationalized using point group theory.

References

- [1] A. Abedi, N. T. Maitra, E. K. U. Gross, Phys. Rev. Lett. (2010).
- [2] A. J. Jenkins, K. E. Spinlove, M. Vacher, G. A. Worth, and M. A. Robb, J. Chem. Phys. (2018).
- [3] G. A. Worth, I. Burghardt, Chem. Phys. Lett. (2003).
- [4] M. Olivucci, T. Tran, G. A. Worth, and M. A. Robb, J. Phys. Chem. Lett. (2021).
- [5] T. Tran, G. A. Worth, and M. A. Robb, Commun. Chem. (2021).

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Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 38

Time: May 25, 2022 10:00 AM Eastern Time (US and Canada)

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