VISTA Seminar

Seminar 46

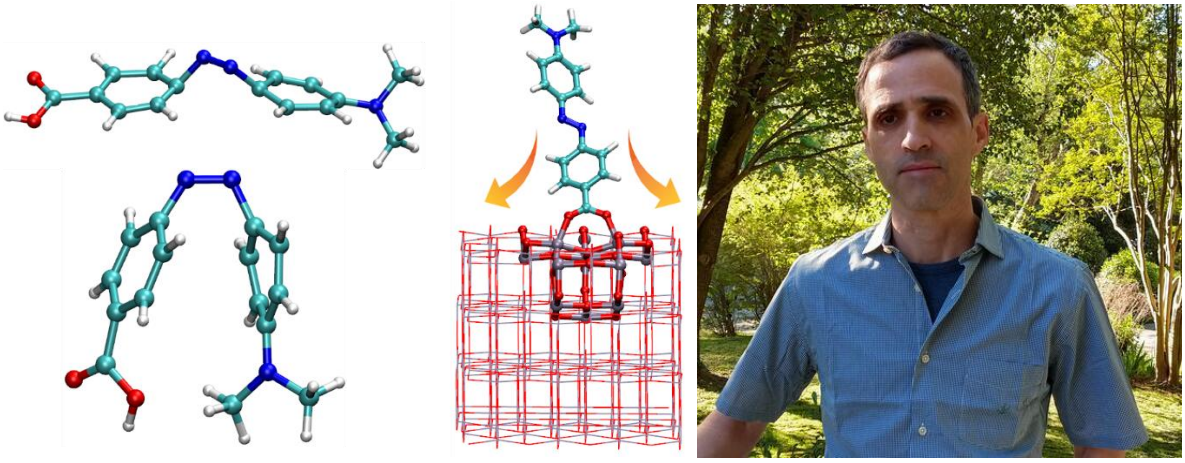
November 30, 2022

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:

Photoinduced Coupled Electronic-Structural Dynamics of Molecular Systems

Luis G. C. Rego
Department of Physics,
Universidade Federal de Santa Catarina, Florianópolis, SC, Brasil
Email: luis.gc.rego@gmail.com or luis.guilherme@ufsc.br



Charge transfer and electronic excitation dynamics are ubiquitous in photochemistry. They constitute the underlying mechanisms for electron transfer reactions, light-harvesting in natural and artificial molecular structures, energy transduction phenomena, and many other processes in atomic, molecular physics, chemistry and biology. They are often influenced by the non-adiabatic coupling between electronic and nuclear degrees of freedom, so that dynamics simulations on a single Born-Oppenheimer potential energy surface (PES), usually in the ground-state, cannot fully describe them. In this talk I describe a hybrid QM-MM self-consistent method that incorporates non-adiabatic electronic quantum dynamics into molecular mechanics, for simulations of large scale atomistic structures subject to complex structural deformations [1-3]. Simulations are carried out within the framework of the self-consistent Ehrenfest (SE) method and the Coherent Switching with Decay-of-Mixing (CSDM) method proposed by Truhlar and collaborators [4]. The CSDM method improves on both the SE and trajectory surface hopping methods, as it introduces decoherence into the electronic non-adiabatic dynamics as a result of the nuclear motion. The hybrid QM-MM implementation of these methods are suited for materials science and biochemistry simulations. We present results for photo-induced isomerization and charge transfer driven vibrational relaxation of photo-chromic molecular systems.

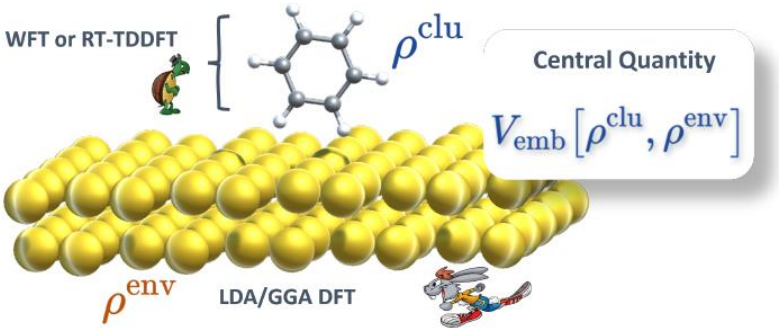
References:

[1] J. Phys. Chem. C, **120**, 27688 (2016)
[2] J. Phys. Chem. Lett., **9**, 5926 (2018)
[3] J. Phys. Chem. C, **123**, 5692 (2019)
[4] J. Chem. Theory Comput., **16**, 4098 (2020)

Density Functional Theory Based Embedding for Molecular and Periodic Systems Using Gaussian Basis Functions

Manas Sharma, Marek Sierka

Otto Schott Institute of Materials Research, Friedrich Schiller University of Jena, L¨obdergraben 32, 07743 Jena, Germany.
E-mail: manas.sharma@uni-jena.com and marek.sierka@uni-jena.com



The high computational demand for modeling hybrid systems, such as solvated molecules or molecules adsorbed on a surface, has led to the development of many embedding methods, especially since the region of interest is usually smaller. An implementation of density functional theory-based embedding coupled with wavefunction theory (WFT) methods and real time-time dependent density functional theory (RT-TDDFT) is presented. Its key feature is that it allows treating both periodic and aperiodic systems on an equal footing using an all-electron direct-space representation, by employing Gaussian basis functions. The three flavors of embedding: molecule-in-molecule, molecule-in-periodic, and periodicin-periodic are implemented using embedding potentials based on non-additive kinetic energy density functionals (approximate) and level-shift projection operator (exact). The applicability of (i) WFT-in-DFT embedding, in predicting the ground and excited state properties of the embedded clusters, and (ii) RT-TDDFT-in-DFT, in predicting the absorption spectra, is explored for various test systems.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 46
Time: Nov 30, 2022 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting
https://buffalo.zoom.us/j/98599048260?pwd=Szd2YVJTRng3akoxeFR1emJ0ak5LZz09

Meeting ID: 985 9904 8260
Passcode: 546879
One tap mobile
+16465588656,,98599048260#,,,,*546879# US (New York)
+13017158592,,98599048260#,,,,*546879# US (Washington DC)

Dial by your location
- +1 646 558 8656 US (New York)
- +1 301 715 8592 US (Washington DC)
- +1 312 626 6799 US (Chicago)
- +1 253 215 8782 US (Tacoma)
- +1 346 248 7799 US (Houston)
- +1 669 900 9128 US (San Jose)

Meeting ID: 985 9904 8260
Passcode: 546879
Find your local number: https://buffalo.zoom.us/u/aVTNHGM8J

Join by SIP
98599048260@zoomcrc.com

Join by H.323
162.255.37.11 (US West)
162.255.36.11 (US East)
115.114.131.7 (India Mumbai)
115.114.115.7 (India Hyderabad)
213.19.144.110 (Amsterdam Netherlands)
213.244.140.110 (Germany)
103.122.166.55 (Australia Sydney)
103.122.167.55 (Australia Melbourne)
149.137.40.110 (Singapore)
64.211.144.160 (Brazil)
69.174.57.160 (Canada Toronto)
65.39.152.160 (Canada Vancouver)
207.226.132.110 (Japan Tokyo)
149.137.24.110 (Japan Osaka)
Meeting ID: 985 9904 8260
Passcode: 546879