

VISTA Seminar

Seminar 16

April 14, 2021

9:30 – 11:00 am EDT / 2:30 – 4:00 pm GMT / 3:30 pm – 5:00 pm Paris

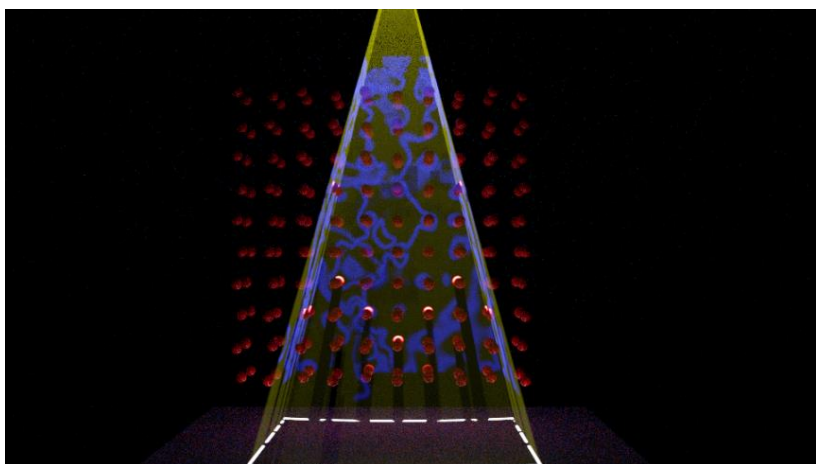
TOC:

1. Presenter 1: Prof. Andre Schleife, University of Illinois, Urbana-Champaign, USA..... page 2
2. Presenter 2: Dr. Momir Mališ, University of Zurich, Switzerland page 3
3. How to connect..... page 4

Electron and ion dynamics in materials due to particle radiation and optical excitation

Andre Schleife

University of Illinois, Urbana-Champaign, Department of Materials Science and Engineering
E-mail: schleife@illinois.edu Phone: +1 (217) 244 0339



Manipulation of matter using particle or laser beams can achieve precisely tuned atomic geometries that are necessary, e.g. to engineer interactions in quantum materials and for fabricating novel electronic devices with nanoscale dimensions. In addition, such beams are also used to characterize and probe properties of materials using by means of electronic and optical excitations. In this talk I will present recent quantum-mechanical first-principles predictions for electron dynamics and the subsequent ionic motion that follows after an initial excitation of the electronic system. Using real-time time-dependent density functional theory we simulated the underlying ultrafast time scales of electron dynamics in semiconductors and metals. Examples include long-lived electronic excitations in proton and laser irradiated MgO that facilitate diffusion of oxygen vacancies. We compare these bulk simulations to proton and laser irradiated aluminum surfaces, for which we quantify electron emission, charge capture, and pre-equilibrium electronic stopping effects that are unique to thin films or two-dimensional materials. Limitations and possible extensions of the theoretical description will be included in the discussion.

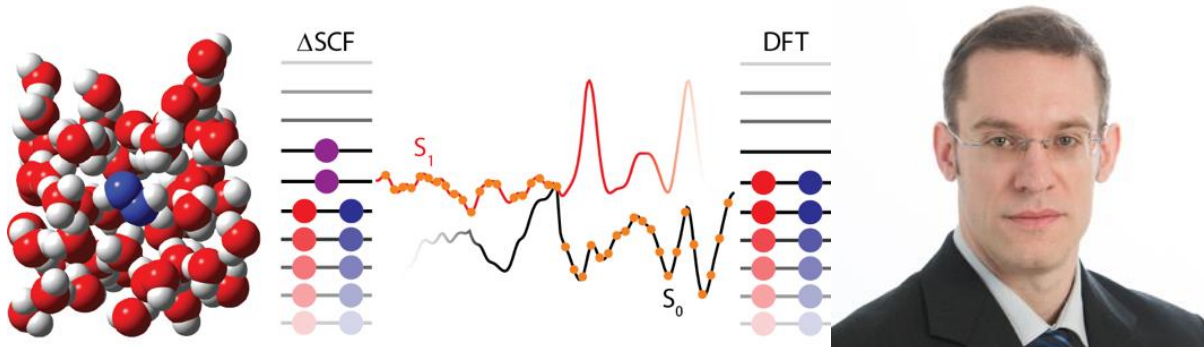
Funding from the Office of Naval Research is gratefully acknowledged N00014- 18-1-2605.

Δ SCF for Efficient Nonadiabatic Molecular Dynamics in Condensed Phase Systems

Momir Mališ, Sandra Luber

University of Zurich, Department of Chemistry, Winterthurerstrasse 190, 8057 Zürich, Switzerland

Email: momir.malis@uzh.ch



Accurate calculation of excited electronic state properties in the condensed phase systems represents the main bottleneck for efficient application of semiclassical nonadiabatic molecular dynamics (NA-MD) methods for investigation of nonadiabatic processes in the condensed phase taking place after photoexcitation. A variational delta self-consistent field (Δ SCF) density functional theory (DFT) based method¹ represents a potential approach to address the aforementioned constraints in addition to perturbative time-dependent density functional theory (TD-DFT). We applied a restricted Kohn-Sham formulation of Δ SCF with constrained and rounded occupation numbers for NA-MD and employed TD-DFT to aid in excited state SCF convergence and provide guess electronic state densities.² By utilizing the combined Gaussian and plane waves approach with periodic boundary conditions the method is easily applicable to full atomistic DFT simulations of condensed phase and it can be combined with subsystem density embedding to further expand its capabilities. We applied it to study the nonradiative deactivation mechanism of photoexcited diimide in water solution, and show the advantages and disadvantages of such a pragmatic new technique for efficient simulation of nonadiabatic processes in the condensed phase.³

1. Pradhan, Sato, Akimov: Non-adiabatic molecular dynamics with Δ SCF excited states *J. Condens. Matter Phys.* **30** (2018) 484002
2. Mališ, Luber: Trajectory Surface Hopping Nonadiabatic Molecular Dynamics with Kohn-Sham Δ SCF for Condensed-Phase Systems *J. Chem. Theory Comput.* **16** (2020) 4071
3. Mališ, Luber: Δ SCF with Subsystem Density Embedding for Efficient Nonadiabatic Molecular Dynamics in Condensed-Phase Systems *J. Chem. Theory Comput.* **17** (2021) 1653

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 16

Time: Apr 14, 2021 09:30 AM Eastern Time (US and Canada)

Join Zoom Meeting

<https://buffalo.zoom.us/j/97994681741?pwd=ZUNrZDgrSGF2eDJMQWpaQUtXVnk81QT09>

Meeting ID: 979 9468 1741

Passcode: 917509

Join by SIP

97994681741@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: 979 9468 1741

Passcode: 917509