VISTA

VISTA Seminar

Seminar 16

April 14, 2021

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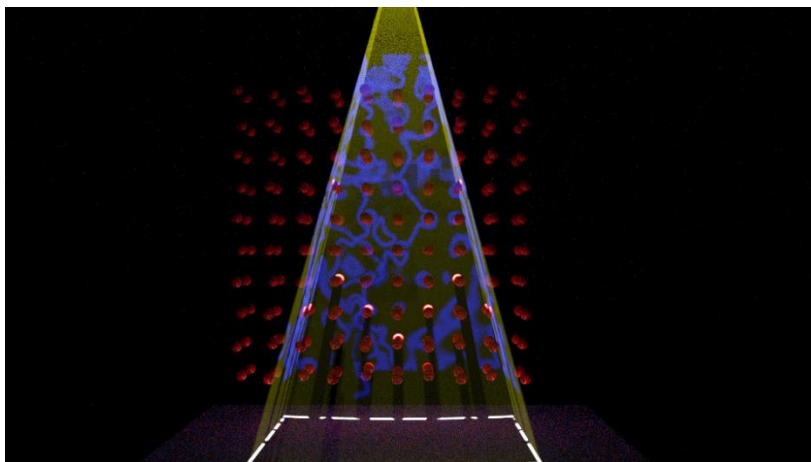
TOC:

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

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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.
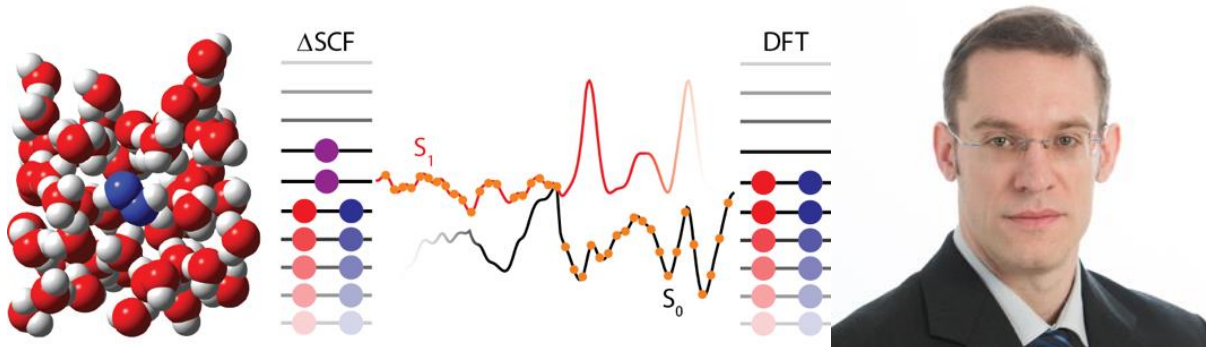
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ΔSCF for Efficient Nonadiabatic Molecular Dynamics in Condensed Phase Systems

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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 (ΔSCF) density functional theory (DFT) based method[1] 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 ΔSCF 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 ΔSCF excited states *J. Condens. Matter Phys.* **30** (2018) 484002
2. Mališ, Luber: Trajectory Surface Hopping Nonadiabatic Molecular Dynamics with Kohn-Sham ΔSCF for Condensed-Phase Systems *J. Chem. Theory Comput.* **16** (2020) 4071
3. Mališ, Luber: ΔSCF 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)

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