EXCITED ELECTRONS IN SEMICONDUCTORS: DIELECTRIC SCREENING AND NON-ADIABATIC DYNAMICS

Dr. André Schleife

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Thursday Feb. 16

4:00 PM HH 202

Using high-performance super computers, computational materials scientists employ extremely accurate quantum-mechanical approaches to reliably predict materials properties. In particular, many-body perturbation theory is a theoretical framework for theoretical spectroscopy, capable of predicting electronic and optical properties. Real-time time-dependent density functional theory is an accurate approach that is suitable to study the non-adiabatic dynamics of electrons and fast-moving ions. Both techniques provide insight with unprecedented, predictive accuracy.

In this talk I will show how solving the Bethe-Salpeter equation for the optical polarization function allows to understand how free-electron and lattice contributions to dielectric screening impact optical properties. This is illustrated for novel organo-metal halide perovskites and oxides: It will be shown that screening due to free carriers and due to lattice polarizability reduces excitonic effects. Results from many-body perturbation theory and density functional theory also allow us to understand experimental data for semiconductor nanocrystals, leading to an optical spectroscopy-based technique for high-throughput phase identification.

Furthermore, I will show how time-dependent density functional theory allows us to describe non-adiabatic dynamics of electrons and ions for solids that are subject to particle radiation: The fast-moving, time-depending Coulomb potential of the highly energetic projectile ions directly interacts with the electronic system of the target. The ensuing electronic excitations are an efficient energy-loss mechanism for the projectile, also known as electronic stopping. I will report on Ehrenfest molecular dynamics simulations of this energy transfer and the emerging ultrafast electron dynamics. The influence of surfaces is explored and quantified, which is important, e.g. for helium microscopy and focused-ion beam sample manipulation and characterization.

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André Schleife is a Blue Waters Assistant Professor in the Department of Materials Science and Engineering at the University of Illinois at Urbana-Champaign. He obtained his Diploma and Ph.D. at Friedrich-Schiller-University in Jena, Germany for his theoretical work on transparent conducting oxides. Before he started at UIUC he worked as a Postdoctoral Researcher at Lawrence Livermore National Laboratory on a project that aimed at a description of non-adiabatic electron ion dynamics. His research revolves around excited electronic states and their real-time dynamics in various materials using accurate computational methods and making use of modern super computers. He also focuses on understanding the interaction between excited electrons and ions.

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