

Spring 2019 Joint Colloquium

Materials Department & Materials Research Laboratory

Professor André Schleife

Department of Materials Science and
Engineering
University of Illinois at Urbana-Champaign

Friday, May 24th, 2019
11:00 am, ESB 1001



Excited electronic states and their ultrafast dynamics: Pushing towards materials engineering and design

Electronic excitations and their time dynamics are at the foundation of how we use and probe matter. Recent experimental advances allow us to do so with unprecedented accuracy and time resolution, however, their interpretation relies on solid theoretical understanding. This can be provided by first-principles theoretical-spectroscopy, based on many-body perturbation theory and time-dependent density functional theory. In this talk, I will illustrate recent successful examples for how these electronic-structure methods lead to deep understanding, e.g. of light absorption of organo-metal halides and the enhancement of defect diffusion by hot electrons under radiation conditions. While these first-principles simulation techniques allow for predictive accuracy and excellent agreement with experiment, they rely on approximations, and I will illustrate our recent efforts of developing better theoretical understanding of dielectric screening physics and how to bridge time scales from ultrafast electron dynamics to atomic diffusion. Finally, I will describe how incorporating online databases into computational research on excited electronic states can side-step the problem of high computational cost to facilitate materials design.

Bio

André Schleife is a Blue Waters Assistant Professor in the Department of Materials Science and Engineering at the University of Illinois at Urbana-Champaign. Research in his group revolves around excited electronic states and their real-time dynamics in various materials using accurate computational methods and making use of modern super computers. Schleife obtained his Diploma and Ph.D. at Friedrich-Schiller-University in Jena, Germany for theoretical and computational 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. He received the NSF CAREER award, the ONR YIP award, and the ACS PRF doctoral new investigator award.

<http://schleife.matse.illinois.edu/index.html>

Hosted by Chris Van de Walle.