UC RIVERSIDE UNIVERSITY OF CALIFORNIA | Materials Science and Engineering

Winter 2020 COLLOQUIUM SPEAKER

Electronic excitations: Optical properties, femto-second dynamics, and materials selection

Using and probing materials oftentimes involves techniques that create or analyze electronic excited states. Recent experimental advances allow studying these, as well as their femto-second real-time dynamics, with unprecedented accuracy and high time resolution. Interpretation of such experiments, however, relies on solid theoretical and fundamental understanding. First-principles theoretical-spectroscopy, e.g. based on many-body perturbation and time-dependent density functional theory, can provide such an accurate description, as I will illustrate in this talk for several recent, successful examples: Using these electronic-structure methods, we facilitated optical crystal-structure identification, provided deep understanding of light absorption for organo-metal halides, and explored the enhancement of defect diffusion by hot electrons under radiation conditions. Since the predictive accuracy of these techniques depends on physical and numerical approximations, I will also discuss our efforts in addressing deficiencies, such as the description of dielectric screening and explain how we bridge multiple time scales from ultrafast electron dynamics to atomic diffusion. In addition, I will describe how incorporating online databases into computational research on excited electronic states can side-step the problem of high computational cost associated with first-principles simulations and, thus, facilitate materials selection for semiconductor heterojunctions.

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Dr. André Schleife

Assistant Professor,
Materials Science & Engineering,
University of Illinois

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, using and implementing accurate computational methods, and making use of modern high-performance 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. He then worked as a Postdoctoral Researcher at Lawrence Livermore National Laboratory on a description of non-adiabatic electron-ion dynamics. He received the NSF CAREER award, the ONR YIP award, and is an ACS PRF doctoral new investigator. André is member of the Executive Committee of the Division of Computational Physics of the APS, editor for a journal, and actively organizes national and international schools, workshops, and tutorials to advance the community around cutting-edge first-principles simulations of materials.

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