MAR16-2015-020277

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

Hot Electron Dynamics at Semiconductor-Molecule Interfaces: Insights from First-Principles Dynamics Simulation

YOSUKE KANAI, University of North Carolina at Chapel Hill

Quantum dynamics of excited electrons is fundamental to functionalities of semiconductor-molecule interfaces that are an integral part of various solar energy conversion and opto-electronic technologies. Thus, developing a predictive and quantitative understanding of the electron dynamics at the atomistic level for such complex interfaces is of great interest. In this talk, I will discuss our recent effort on addressing several challenges in understanding how atomistic features such as surface defects influence these electron dynamical processes. We tackle this problem theoretically by employing a first-principles simulation approach that synergistically combine fewest switches surface hopping, many-body perturbation theory, and first-principles molecular dynamics. New findings from the first-principles simulation will be discussed in the context of a larger effort within Solar Fuels EFRC at UNC Chapel Hill. I will also discuss how the results from atomistic theories pose a conceptual challenge when characterizing these interfacial electron processes for these complex interfaces using a simple kinetic model.