

Abstract Submitted  
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**First-Principles Simulation of Hot Electron Dynamics at Silicon-Molecule Interfaces** LESHENG LI, YOSUKE KANAI, Univ of NC - Chapel Hill, KANAI GROUP TEAM — Hot carrier relaxation process at an interface between semiconductor and molecular ligands is of great importance for a number of technological applications ranging from photo-electrochemical cells to quantum-dot light emitting diodes. Although a number of spectroscopic experiments suggest important role of molecular ligands at surface in the hot carrier relaxation, a quantitative understanding has not been developed. We investigate the hot electron relaxation process through synergetic use of first-principles molecular dynamics (FPMD), fewest switch surface hopping (FSSH) algorithm, and GW calculations. Using FSSH stochastic dynamics simulation based on non-adiabatic couplings from FPMD and quasi-particle energy level alignment at the interface, we investigate the role of molecular passivation at silicon (111) surface as a representative example. We will discuss how different types of molecules influence the relaxation process and elucidate important factors controlling the relaxation time scale.

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