

Abstract Submitted  
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**First-Principles Investigation of Hot Carrier Relaxation in Quantum-Dots** KYLE REEVES, LESHENG LI, YOSUKE KANAI, Univ of NC - Chapel Hill — A combination of fewest-switches surface hopping simulations and Kohn-Sham (KS) density functional theory allows us to obtain key insights into hot carrier relaxation processes in materials. In particular, a first-principles approach allows us to investigate the influence of atomistic details such as the surface chemistry on the relaxation process in quantum dots. At the same time, the accuracy of the KS single-particle energies impacts the simulated non-adiabatic relaxation rate. Using a small gold nanocluster as a model system, we investigate how relaxation rates are influenced by the single-particle energies by considering a hybrid functional in DFT and the GW approximation.

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