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Exploring the Influence of the Chemical Passivation on Electron Relaxation in Silicon Quantum Dots Using First-Principles Surface Hopping Methods YOSUKE KANAI, KYLE REEVES, University of North Carolina at Chapel Hill, ANDRE SCHLEIFE, Lawrence Livermore National Laboratory — The generation of hot carriers in nano-materials is an exciting phenomenon that could potentially increase the efficiency of photovoltaic and photo-electrochemical cells significantly. The electron relaxation dynamics of a system is related to both the electronic and phononic contributions. Given that both of these contributions are ultimately derived from the electronic structure of a system, chemical substitutions may play a significant role in augmenting and controlling the electron relaxation dynamics in nano-materials. With greater insight into the phenomenon from the first-principles theory, engineering new nano-materials with novel opto-electronic properties via a chemical functionalization of its surface becomes a more realistic avenue. A first-principles surface hopping approach based on density functional theory calculations is used to elucidate the relaxation dynamics in silicon quantum-dots. We explore how varying the passivating species on silicon quantum dots influences the electron relaxation dynamics in the system. The two systems considered here are hydrogen-passivated and fluorine-passivated silicon quantum dots. We present a detailed analysis of the electron relaxation dynamics in these nano-materials.

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