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Nonadiabatic electron-phonon coupling and hot carrier relaxation in amorphous silicon TAE-HO PARK, SungKyunKwan Univ. Korea, MARK LUSK, Colorado School of Mines, United States — Energy and optoelectronics applications for quantum confined silicon dots generally require an efficient means of collecting and distributing charge carriers. This has led us to consider quantum dots encapsulated within a hydrogenated amorphous silicon matrix which plays a critical role in photon collection, hot carrier cooling and transport. A theoretical framework to quantify the phonon assisted charge transfer and the carrier relaxation rates in both amorphous and crystalline Si has been developed based on nonadiabatic coupling (NAC). The vibrational part in these rates is obtained analytically using an extended Frank-Condon formulation, while the electronic part is numerically calculated using a combination with Time-Dependent Density Functional Theory (TD-DFT) and Density Functional Perturbation Theory (DFPT). We use this new methodology to predict cooling rates and transport mobilities for amorphous silicon, and these predictions compare well with experimental measurements. The approach is then extended to calculate analogous values for nanocrystalline silicon, allowing us to propose a likely conduction mechanism for carrier transport through such mixed amorphous/crystalline materials.

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