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The Influence of Phonons and Surface Termination on Optical Transitions in Small Silicon Quantum Dots and Implications for Exciton Transport[1] ZHIBIN LIN, Department of Physics, Colorado School of Mines, ALBERTO FRANCESCHETTI, National Renewable Energy Laboratory, MARK LUSK, Department of Physics, Colorado School of Mines — Bulk silicon is an indirect-gap semiconductor, and radiative recombination can proceed only through phonon assistance. Recent experiments suggest, though, that fast, zero-phonon, pseudo-direct transitions occur in silicon quantum dots (Si QDs) as a result of quantum confinement. On the other hand, previous theoretical studies based on tight-binding and effective mass methodologies yield contradictory conclusions on the degree to which phonons play a role in radiative recombination within Si QDs. The resolution of this issue has important repercussions for ways in which Si QDs can be incorporated into future photovoltatic designs. This also has implications as to how QD size, phonons, and surface ligands collectively influence exciton transport. Density functional theory, in concert with a phonon-corrected version of Fermi's Golden Rule, is used to investigate the degree to which phonons influence the rate of optical transitions in Si QDs and to elucidate how the role of phonons changes with dot size and surface termination (H, CH3, and OH). The results are compared with available experimental data and those of previous calculations. In addition, the implications for phonon-assisted exciton transport dynamics within Si QD assemblies will be discussed.

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