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Free-Carrier Absorption in Silicon from First Principles[1] GUANGSHA SHI, EMMANOUIL KIOUPAKIS, Univ of Michigan - Ann Arbor — The absorption of light by free carriers in semiconductors such as silicon results in intraband electron or hole excitations, and competes with optical transitions across the band gap. Free-carrier absorption therefore reduces the efficiency of optoelectronic devices such as solar cells because it competes with the generation of electron-hole pairs. In this work, we use first-principles calculations based on density functional theory to investigate direct and phonon-assisted free-carrier absorption in silicon. We determine the free-carrier absorption coefficient as a function of carrier concentration and temperature and compare to experiment. We also identify the dominant phonon modes that contributing to phonon-assisted free-carrier absorption processes, and analyze the results to evaluate the impact of this loss mechanism on the efficiency of silicon solar cells.

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