Electronic and Optical Properties of Novel Phases of Silicon and Silicon-Based Derivatives

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— Recent discoveries of two novel phases of silicon, Si$_{20}$ and Si$_{24}$, lead to promises of quasi-direct band gap silicon crystals that are capable of complementing indirect-gap diamond cubic silicon for use in the solar cell industry. This work studies the quasiparticle excitations and optical spectra of these two structures, Si$_{20}$ and Si$_{24}$, assessing their suitability for use as photovoltaic materials. We carry out ab initio GW and GW-BSE calculations for the quasiparticle excitations and optical spectra, respectively, including self-energy and electron-hole interaction effects. This work was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory’s NERSC facility.

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