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Electronic and optical properties of body-centered tetragonal Si and Ge[1] BRAD D. MALONE, STEVEN G. LOUIE, MARVIN L. COHEN, Department of Physics, University of California, Berkeley, and Materials Science Division, Lawrence Berkeley National Laboratory — We present a first-principles calculation of the quasiparticle and optical excitation spectra of recently predicted silicon and germanium polytypes in the bct structure. The quasiparticle spectra, calculated within the GW approximation, predicts that both silicon and germanium in the bct structure are small band gap materials with direct gaps of 1.1 eV and 0.79 eV, respectively. The optical spectra is evaluated by solving the Bethe-Salpeter equation taking into account electron-hole interactions. We then make comparison to the cubic phases of Si and Ge which suggest the possible utility of the bct phases in photovoltaic applications.

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Brad D. Malone
UC Berkeley

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