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Electronic Structure of Silicon Phases Resulting from Decompression from β-Sn[1] BRAD MALONE, JAY SAU, MARVIN COHEN, UC Berkeley, Lawrence Berkeley National Laboratory — We present an *ab initio* study of the electronic structure of the silicon phases that result from decompression from the metallic β-Sn phase, namely the BC8 (Si III), the hexagonal diamond (Si IV), the R8 (Si XII), and the yet unobserved ST12 phases. To correct for the inadequacies in the DFT-LDA quasiparticle energy spectra we employ quasiparticle corrections with the framework of the GW approximation. In doing so we find that the R8 phase should be semiconducting at lower pressures We also analyze the effect of strain and doping on these materials in an attempt to find novel applications for these phases, from high-mobility semiconductors to superconductivity.

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