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A new metastable phase of silicon in the *Ibam* structure BRAD D. MALONE, MARVIN L. COHEN, Department of Physics, University of California, Berkeley, and Materials Science Division, Lawrence Berkeley National Laboratory — In a study aimed at finding new useful forms of silicon, we use an *ab initio* random structure searching (AIRSS) method to identify a new phase of silicon in the *Ibam* structure. The *Ibam* phase is found to be semimetallic within density functional theory with a small band overlap, and it is expected that quasiparticle corrections using the GW approximation would yield a semiconducting state with a small band gap. Calculation of the lattice dynamics reveals that the structure is locally stable. Enthalpy-pressure relations are calculated for the *Ibam* structure as well as all other known Si structures, including the previously predicted phases st12 and bct. These results indicate that *Ibam* silicon is metastable over the pressure range considered. Calculated coexistence pressures of the other known phase transitions are in good agreement with experimental observation.

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