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***Ab initio* study of the optical properties of Si-XII**¹ BRAD MALONE, JAY SAU, MARVIN COHEN, Department of Physics, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — We present a first-principles calculation of the optical excitation spectrum of Si-XII, a high-pressure, metastable phase of silicon in the R8 structure. Recent calculations of the quasiparticle spectrum have shown Si-XII to be semiconducting with a small, indirect band gap. In this paper we solve the Bethe-Salpeter equation (BSE) to obtain the optical spectrum of this material. We then compare our calculated optical spectrum with experimental data for other forms of silicon commonly used in photovoltaic devices. These include cubic, polycrystalline, and amorphous forms of silicon. We find that the calculated values of the optical functions relevant to photovoltaic absorption in Si-XII show greater overlap with the incident solar spectrum than those found in these other silicon phases.

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Brad Malone
Department of Physics, University of California, Berkeley and
Materials Sciences Division, Lawrence Berkeley National Laboratory

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