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Electronic and Optical Properties of Novel Phases of Silicon and Silicon-Based Derivatives CHIN SHEN ONG, SANGKOOK CHOI, STEVEN LOUIE, University of California at Berkeley — The vast majority of solar cells in the market today are made from crystalline silicon in the diamond-cubic phase. Nonetheless, diamond-cubic Si has an intrinsic disadvantage: it has an indirect band gap with a large energy difference between the direct gap and the indirect gap. In this work, we perform a careful study of the electronic and optical properties of a newly discovered cubic-Si_{20} phase of Si that is found to sport a direct band gap. In addition, other silicon-based derivatives have also been discovered and found to be thermodynamically metastable. We carry out *ab initio* GW and GW-BSE calculations for the quasiparticle excitations and optical spectra, respectively, of these new phases of silicon and silicon-based derivatives. 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 and the NSF through XSEDE resources at NICS.

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