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Real-Space Analysis of the Optical Absorption in Alternative Phases of Silicon CHIN SHEN ONG, Department of Physics, UC Berkeley and Lawrence Berkeley National Lab, SINISA COH, Mechanical Engineering, Materials Science and Engineering, UC Riverside, MARVIN L. COHEN, STEVEN G. LOUIE, Department of Physics, UC Berkeley and Lawrence Berkeley National Lab — We introduce a real-space approach to understand the relationship between optical absorption and crystal structure. This approach is applied to some alternative phases of silicon in addition to the diamond structure, with a focus on the Si_{20} crystal phase as a case study. We find that about 83% of the enhancement in the calculated low-energy absorption in Si_{20} can be attributed to reducing the differences between the on-site energies of the bonding and anti-bonding orbitals as well as to increasing the magnitude of the hopping integrals for specific Si-Si bonds. This work was supported by NSF grant No. DMR-1508412 and the DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility.

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