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Diffusion quantum Monte Carlo study of Silicon Carbide JEREMY MCMINIS, University of Illinois at Urbana Champaign, JEONGNIM KIM, National Center for Supercomputing Applications, FERNANDO REBOREDO, Oak Ridge National Laboratory — Silicon Carbide (SiC) is an important semiconductor used in high temperature electronic applications because of its large excitation energy. We use diffusion quantum Monte Carlo (DMC) to calculate some of its electronic, physical, and optical properties. An analysis of the symmetry of the trial wave-function's single particle orbitals is required because SiC is an indirect gap semiconductor. In order to obtain an upper bound estimate of the energy of the excited state we symmetrize the exciton trial wave-function so that it belongs to an irreducible representation of dimension one. We report results on the equation of state of SiC, and the finite size scaling of the band gap obtained with DMC.

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