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Quantum Monte Carlo examines accuracy of density functional approximations for defects and phase transformations in silicon[1]
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— Silicon displays a variety of interstitial defects limiting device fabrication and performance and shows at least twelve crystallographic phases under pressure. While DFT-determined structures are reliable, defect energies and phase transformation pressures are sensitive to the specific exchange-correlation functional. Diffusion Monte Carlo calculations for silicon defects and phases test the accuracy of the current density-functional approximations LDA, PW91, PBE, and TPSS. Diffusion Monte Carlo predicts the correct cohesive energy of the diamond structure, however, the pressure for the transition to beta-tin is larger than in experiments. The transformation is sensitive to anisotropic stresses; an anisotropy of 2-3 GPa lowers the prediction to agree with experiment. Diffusion Monte Carlo for high-pressure Si phases and interstitial defect clusters shows that relative to diamond Si the energies of phases and defects are underestimated by DFT.

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