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Accurate band gaps of semiconductors and insulators from Quantum Monte Carlo calculations ROMAN NAZAROV, RANDOLPH HOOD, MIGUEL MORALES, LLNL — Ab initio calculations are useful tools in developing materials with targeted band gaps for semiconductor industry. Unfortunately, the main workhorse of ab initio calculations – density functional theory (DFT) in local density approximation (LDA) or generalized gradient approximation (GGA) underestimates band gaps. Several approaches have been proposed starting from empirical corrections to more elaborate exchange-correlation functionals to deal with this problem. But none of these work well for the entire range of semiconductors and insulators. Deficiencies of DFT as a mean field method can be overcome using many-body techniques. Quantum Monte Carlo (QMC) methods can obtain a nearly exact numerical solutions of both total energies and spectral properties. Diffusion Monte Carlo (DMC), the most widely used QMC method, has been shown to provide gold standard results for different material properties, including spectroscopic constants of dimers and clusters, equation of state for solids, accurate descriptions of defects in metals and insulators. To test DMC's accuracy in a wider range of semiconductors and insulators we have computed band gaps of several semiconductors and insulators. We show that DMC can provide superior agreement with experiment compared with more traditional DFT approaches including high level exchange-correlation functionals (e.g. HSE).

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