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Advances in the application of diffusion Monte Carlo to solids
L. SHULENBURGER[1], T.R. MATTSSON, Sandia National Laboratories — The need for high fidelity electronic structure calculations has catalyzed an explosion in the development of new techniques. Improvements in DFT functionals, many body perturbation theory and dynamical mean field theory are starting to make significant headway towards reaching the accuracy required for a true predictive capability. One technique that is undergoing a resurgence is diffusion Monte Carlo (DMC). The early calculations with this method were of unquestionable accuracy (providing a valuable reference for DFT functionals) but were largely limited to model systems because of their high computational cost. Algorithmic advances and improvements in computer power have reached the point where this is no longer an insurmountable obstacle. In this talk I will present a broad study of DMC applied to condensed matter (arXiv:1310.1047). We have shown excellent agreement for the bulk modulus and lattice constant of solids exhibiting several different types of binding, including ionic, covalent and van der Waals. We will discuss both the opportunities for application of this method as well as opportunities for further theoretical improvements.

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