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High throughput quantum Monte Carlo calculations of material formation energies KAYAHAN SARITAS, Massachusetts Institute of Technology, Department of Materials Science and Engineering, TIM MUELLER, Johns Hopkins University Whiting School of Engineering, LUCAS WAGNER, University of Illinois Urbana Champaign, Physics Department, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology — High throughput calculations based on approximate density functional theory (DFT) methods have been widely implemented in the scientific community although depending on both the properties of interest as well as particular chemical/structural phase space, accuracy even for correct trends remains a key challenge for DFT. In this work, quantum Monte Carlo calculations are applied using a recipe developed for a high throughput computing environment. We compare our approach to different DFT methods as well as different pseudopotentials, showing that errors in QMC calculations can be progressively improved especially when correct pseudopotentials are used. We show that using this simple automated recipe, QMC calculations can outperform DFT calculations over a wide set of materials. We show that out of 21 compounds tested, chemical accuracy has been obtained in formation energies of 11 structures using our QMC recipe, compared to none using DFT calculations.

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