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Quantum Monte Carlo for Materials Design TIM MUELLER, Johns Hopkins University, LUCAS WAGNER, University of Illinois at Urbana-Champaign, JEFFREY GROSSMAN, Massachusetts Institute of Technology — The accurate calculation of formation energies is critical to evaluating the stability and chemical reactivity of newly designed materials. Comprehensive databases of formation energies can be used to screen materials for stability before they have been synthesized, but the reliability of such databases depends on the accuracy of the data they contain. Quantum Monte Carlo (QMC) is a highly accurate method that can calculate the formation energies a wide variety of chemical substances, including molecules and metals. The wide applicability of QMC calculations is made possible in part by the fact that the cost of a QMC calculation scales roughly linearly with system size when calculating energies per atom. The accuracy of QMC comes at significant computational cost, but it scales nearly linearly with the number of processors up to a large numbers of processing cores, making it well-suited for large, highly parallel computers. As the initial step towards developing a database of accurate formation energies calculated using QMC, we demonstrate how automated QMC calculations can be used to accurately calculate the formation energies of a variety of different materials.

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