

Abstract Submitted
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Quantum Monte Carlo for Materials Design TIM MUELLER, LUCAS WAGNER, JEFFREY GROSSMAN, Massachusetts Institute of Technology — When designing new materials it is important to have an accurate measure of the material's formation energy to assess thermodynamic stability and chemical activity. Computational materials science holds the potential to accurately predict formation energies, but widely-used methods such as density functional theory often yield large errors when calculating energy differences between compounds with significantly different electronic structures. More accurate quantum chemical methods tend to scale poorly with system size, making it infeasible to apply them to many materials. One exception is quantum Monte Carlo (QMC), which effectively scales linearly or better with system size when calculating formation energy per atom. QMC scales perfectly with the number of processors, making it ideally positioned to take advantage of the rapidly growing core count in central and graphics processing units. It has been shown that quantum Monte Carlo can successfully predict formation energies for some solid state materials, but a broad assessment has been lacking. We have run QMC calculations on a variety of different materials for which high-quality experimental data exists. We present data on the cost and accuracy of QMC, providing insight into the role QMC will play in materials design.

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