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Quantum Monte Carlo calculations in solids: downfolded Hamiltonians and multiple-projector pseudopotentials[1] FENGJIE MA, WIRAWAN PURWANTO, SHIWEI ZHANG, HENRY KRAKAUER, College of William and Mary — Accurate and efficient treatment of core electrons presents a significant challenge in many-body calculations. We discuss two approaches for addressing this problem. In the first, a systematic downfolding method is developed for extended systems, which allows many-body calculations to operate on a simpler and systematically improvable Hamiltonian, while retaining material-specific properties. As a by-product, pseudopotential errors are essentially eliminated using a frozen-core treatment[2]. Dramatic savings of computational cost and excellent accuracy are achieved for a range of solids with auxiliary-field quantum Monte Carlo (AFQMC). With this method, we determine the spin gap in NiO, a challenging material with strong electron correlation effects. In the second approach, we have implemented the recently developed multiple-projector pseudopotentials[3] into planewave based AFQMC (pw-AFQMC), which improves transferability and leads to much smaller planewave cutoff, hence less computational cost, in the pw-AFQMC calculations. We will present comparative studies of the NaCl equation of state between the two approaches. Results will also be presented for more strongly correlated metal systems.

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[2]W. Purwanto et al., JCTC 9, 4825 (2013)
[3]D. R. Hamann, PRB 88, 085117 (2013)

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