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Downfolding calculations in solids by auxiliary-field quantum Monte Carlo[1] FENGJIE MA, WIRAWAN PURWANTO, SHIWEI ZHANG, HENRY KRAKAUER, College of William and Mary — We present a recent development in *ab initio* auxiliary-field quantum Monte Carlo (AFQMC) [2] calculations of solid systems using downfolded Hamiltonians. For a given system, the many-body downfolded Hamiltonian is expressed with respect to a truncated basis set of Kohn-Sham orbitals, which are obtained from a high-quality density-functional calculation. This approach allows many-body calculations to treat a much simpler Hamiltonian while retaining material-specific properties. Typical size of the basis set is more than an order of magnitude smaller than the original (the number of plane-waves), leading to large savings in AFQMC computation. The Hamiltonians are systematically improvable and allow one to dial, in principle, between the simplest model and the full Hamiltonian. As a by-product of this approach, pseudopotential errors can essentially be eliminated [3]. The method is demonstrated by calculating the lattice constant and bulk modulus of solids, including classic semiconductors (Si and diamond), an ionic insulator (NaCl), and metallic systems (Na and Al).

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[2]S. Zhang and H. Krakauer, Phys. Rev. Lett. **90**, 136401 (2003)
[3]W. Purwanto, S. Zhang, H. Krakauer, J. Chem. Theory Comput. **9**, 4825 (2013)

Fengjie Ma
College of William and Mary

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