

Localized and Randomized Linear-Scaling Algorithms for Electronic Structure

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Most linear-scaling algorithms for electronic structure rely on localization of the density matrix [Rev. Mod. Phys. **71**, 1085 (1999)]. They work well for insulators and high-temperature metals that exhibit strong localization but poorly for low-temperature metals with weak localization. More recent stochastic linear-scaling algorithms [Phys. Rev. Lett. **111**, 106402 (2013)] do not depend on localization but converge slowly in the number of statistical samples. We attempt to improve the efficiency of linear-scaling algorithms by combining localized and randomized algorithms. We restrict statistical sampling to the small residual error in a localized density matrix approximation to reduce sampling variance. A variety of algorithms are compared, using both polynomial and rational approximations of the Fermi-Dirac distribution. We apply these algorithms to a series of rhombicuboctahedral copper clusters using the NRL tight-binding model [Phys. Rev. B **63**, 224106 (2001)].

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