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Overcoming the cubic-scaling bottleneck: linear-scaling density functional theory

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ABSTRACT

Electronic structure calculations based on Density Functional Theory (DFT) have been remarkably successful in describing material properties and behavior. In conventional formulations and implementations of DFT, the orthogonality constraint on the orbitals results in a cubic-scaling with respect to the number of atoms. The inherent nonlocality of such approaches also makes them unsuitable for high performance computing. Consequently, the length and time scales for which DFT is practical is severely restricted. In this discussion, earlier and current efforts of the speaker to overcome the aforementioned limitations will be discussed. In particular, the presentation will focus on the development of (i) linear-scaling DFT methods, including those based on purification, spectral quadrature and maximally localized Wannier functions; (ii) a better than linear-scaling technique to coarse-grain DFT, whereby crystal defects can be accurately and efficiently studied. The discussion will conclude with a discussion on possible future directions.