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Low-order scaling methods in density functional theories

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Density functional theories (DFT) have been widely used in chemistry and condensed matter physics, and proven to be a versatile theoretical tool in predicting electronic and geometrical properties of molecules and solids. Having the success of DFT in mind, a next challenge is to simulate more realistic systems involving complex interface structures such as Li ion batteries, permanent magnets, and structural materials, for which the interfaces and grain boundaries play a crucial role in determining the performance of devices. Computational models for these systems may consist of several thousand atoms at least, and oversimplified models may lose fundamental physical processes determining the performance of devices. However, such a simulation tends to be hampered by the computational complexity of DFT calculations which intrinsically scales as O(N3), where N is the number of atoms in the system under investigation. Here, we report our development of low-order scaling methods in DFT based on quantum nearsightedness of electron, whose computational scaling is lower than the cube of the number of atoms N [1-5,13], towards realistic large-scale simulations. An approximate O(N) method based on a Krylov subspace technique [2] and a numerimcally exact low-order scaling method [4] will be introduced in details together with illustrative applications [8-12]. It will be also shown that the idea based on the quantum nearsightedness can be applied to developments of an O(N) non-equibrium Green's function (NEGF) method and a nearly exact exchange functional [5]. Furthermore, a novel parallelization method has been developed based on an inertia tensor moment method to realize large-scale DFT calculations on massively parallel computers typified by the K-computer [6,7].

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