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Functional minimization scheme for first-principles electronic structure calculations with bi-orthogonal interpolating wavelets WILLIAM GARBER, WEI KU, JAMES DAVENPORT, Brookhaven National Lab, DMITRI VOLJA, MIT, Brookhaven National Lab — A new development of a first-principles electronic method will be presented based on direct energy functional minimization and a bi-orthogonal wavelet basis set. The employment of a bi-orthogonal basis allows systematically controlled accuracy while benefiting from compact support that allows O(N) algorithms. Furthermore, utilization of the interpolating nature of wavelets, together with the effectiveness of the multi-resolution of wavelets enables very efficient calculation without compromising accuracy. By avoiding solving an eigenvalue equation as in the standard Kohn-Sham framework, the method is easily extended to parallel algorithms, and allows simple implementation of various non-local functionals. In the case of crystals, our method gives the solution directly as a set of Wannier functions, further utilizing their sparseness. This new development is ideal for easy implementation and accurate systematic benchmarking of various modern functionals, and holds the potential to attack very large systems such as nano-materials.

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