Potentialities of Wavelet formalisms for large-scale DFT calculations and beyond

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The BigDFT software package implements since few years a linear scaling Kohn- Sham density functional theory (LS-DFT) optimization algorithm based on Daubechies wavelets, where a minimal set of localized support functions are optimized in situ and therefore adapted to the physico-chemical properties of the system under investigation.
One key factor influencing the accuracy and cost of DFT is the choice of basis set, where minimal, localized basis sets compete with extended, systematic basis sets. Wavelets offer both locality and systematicity and are thus ideal for representing an adaptive local orbital basis which may be exploited for LS-DFT [1]. One may also make further approximations, e.g. dividing a system into fragments [2] or exploiting underlying repetition of local chemical environments [3], where each approximation may be controlled and quantified. This ability to treat large systems with controlled precision offers the possibility of new types of materials simulations [4].
We will demonstrate the advantages of wavelets as a basis for large scale DFT calculations, as implemented in BigDFT code. We illustrate, from a general perspective, a quantitative method to identify and assess the partitioning of a large quantum-mechanical system into fragments. We will then conclude our discussion by presenting some case-studies among which the example of materials for organic LEDs, showing how our approach may be used to account for environmental and statistical effects on excited state calculations of disordered supramolecular materials [5].

References

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