

DFT LOCALIZED GRID-BASED ORBITALS ON PARALLEL SUPERCOMPUTERS *

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Abstract. Real-space discretizations of the Kohn-Sham equations allow to impose localization constraints on general non-orthogonal orbitals.[1] The computational cost of relaxing the electronic wave functions scales then linearly with the size of the system. However, accurate ab initio calculations based on this approach are still expensive and of practical use on parallel computers only. We discuss the implementation of such methods on various architectures for test systems with more than 2000 orbitals.

REFERENCES

- [1] J.-L. FATTEBERT AND J. BERNHOLC, *Towards grid-based $O(N)$ DFT methods: optimized non-orthogonal orbitals and multigrid acceleration*, Phys. Rev. B, in press.

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