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Linear Scaling First-Principles DFT Calculations with Grid-based Adaptive Orbitals[1] JEAN-LUC FATTEBERT, Lawrence Livermore National Laboratory — As an alternative to the Plane Waves approach for accurate and unbiased Density Functional Theory (DFT) simulations, we have developed a real-space approach which completely avoids use of Fourier transforms. An effective O(N) complexity is achieved by representing the electronic structure as a set of localized nonorthogonal orbitals. The efficiency of the approach has been demonstrated recently for molecular dynamics simulations in the microcanonical ensemble [J.-L. Fattebert and F. Gygi, Phys. Rev. B 73, 115124 (2006)]. Adapting the position of the localization regions on the fly is a key feature to enable accurate MD simulations. In this talk, we will report recent developments in adapting the size of localization regions to improve efficiency and address very general electronic structure problems.

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