GPAW: REAL-SPACE IMPLEMENTATION OF PROJECTOR AUGMENTED WAVE METHOD

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Electronic structure calculations have become valuable tool for materials specific simulations of nanostructures. One of the most succesful frameworks for electronic structure calculations is the density functional theory. We have developed a program package GPAW [1] for density functional calculations using real-space grids together with the projector augmented wave method [2]. The wave functions, densities and potentials are represented on three dimensional uniform real-space grids and a finite difference discretization is used for the Laplacian. Real-space description allows flexible boundary conditions, efficient multigrid algorithms, and efficient parallelization with domain decomposition. However, the wave functions vary rapidly near the nuclei which makes their description on a uniform grid difficult. This problem is solved in projector augmented wave method where accurate all-electron calculations can be performed with smooth wave functions.

We demonstrate the accuracy of the method by calculating atomization energies and bond lengths of small molecules as well as by calculating lattice constants and bulk moduli of some bulk systems. We present also examples about the performance and the parallel scaling of the program. We discuss some future prospects of the method, especially the currently on-going implementation of time-dependent density functional theory

References

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