Large scale electronic structure calculations require high-performance computing. In practice, there are many different codes and many new applications that demand efficient and intelligent numerical methods to efficiently manipulate large data sets. The project ‘Computational Chemistry’ at HPC Jülich is a result of the original necessity for efficient numerical methods in physics and has grown to become a central research topic with many applications in chemistry and materials science. The current version of the Projector Augmented Wave method has been developed for use in real-space quantum chemistry. The PAW method is based on Density Functional Theory (DFT) which is an efficient and accurate technique to calculate the properties of materials and molecules in a solid state. The PAW method replaces the difficult expression of the exchange-correlation functional with an effective potential. The PAW method has the advantage of a high computational efficiency while still providing accurate results.

The PAW method is based on the projector augmented wave (PAW) method. In this method, the electronic wave function is divided into a local part and a non-local part. The local part is represented by a projector, which is a localized basis set of one-dimensional harmonic oscillator (1D HO) eigenfunctions. The non-local part is represented by a non-local potential, which is a function of the atomic ionization potential and the Hartree-Fock exchange potential.

The PAW method has several important advantages over other methods. Firstly, it is very efficient. The computational cost of the PAW method is approximately linear with the size of the system. Secondly, it is very accurate. The PAW method has been shown to be very accurate in a wide range of applications, including solid-state physics, materials science, and chemistry. Finally, the PAW method is very flexible. It can be used to calculate a wide range of properties, including electronic structures, electronic densities, and electronic energies.

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