ACCESSMENT OF ACCURACY AND EFFICIENCY OF PAW DATASETS IN MATERIALS SIMULATIONS

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The community of computational condensed matter researchers have benefited enormously from the work of the developers who maintain high quality public domain software for density functional electronic structure calculations. For example, we use the ABINIT[1] and the QUANTUM ESPRESSO[2] packages interchangeably for structural and energy simulations with the help of atomic datasets generated by our ATOMPAW[3] code. For purposes of asscessment, it is possible to use the same datasets with both ABINIT and QUANTUM ESPRESSO. We find that in the limit of highly converged calculations, it is possible to achieve very close numerical results. However, the approach toward convergence appears to be quite different in the two codes. This is particularly true for density functional perturbation theory calculations used for example in calculating lattice vibrations.

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