

Standard Solid-state Pseudopotentials (SSSP)

The two libraries (SSSP Precision and SSSP Efficiency) cover for each element either the best in class (among many libraries, or generated by us), or occasionally allow for a compromise (either expensive and accurate, or less expensive and a bit less accurate).

The convergence pattern of each element includes for each of the considered family (represented by a color):

- the total number of electrons in the valence, Z ;
- delta value (the error in the equation of state compared with all-electron WIEN2k results, developed by [Cottenier group](#)), at full converged cutoff;
- the largest phonon frequency, ω_{\max} , at the zone boundary (as a number), at full cutoff; and then as a function of wave function cutoff;
- the discrepancy of all phonon frequencies, $\delta\bar{\omega}$, at the zone boundary, with respect to the converged value;
- the convergence of the pressure, δV_{press} , with respect to the converged value;
- the convergence of the cohesive energy, δE_{coh} , with respect to the converged value;
- the convergence of the bands structure, η_{10} and $\max \eta_{10}$ with respect to the converged value.

The suggested wave function cutoff and dual are indicated (the dual is indicated in parentheses). All normconserving psp have a dual of 4 (i.e. $\text{ecutrho}=4*\text{ecutwfc}$); all ultrasoft/PAW have a dual of 8, with the **exception** of Mn and Fe, that have duals of 12. The tests have been made for PBE pseudopotentials using the Quantum ESPRESSO package.

Notes

- We have managed the calculations using AiiDA, an interface to automate, store and share calculations and results.
- All the AiiDA workflows and tools required to run the SSSP protocol are available at <https://github.com/giprandini/sssp-protocol>.

