

Selection Criteria for SSSP

	SSSP Efficiency	SSSP Precision	notes
Phonon frequencies ($\delta\bar{\omega}$)	< 2%	< 1%	(% \rightarrow cm^{-1} if $\omega_{\text{max}} < 100 \text{ cm}^{-1}$)
Cohesive energy (δE_{coh})	< 2 meV/atom	< 2 meV/atom	
Pressure (δV_{press})	< 1%	< 0.5%	in terms of volume differences
Band structure (η_{10})	< 10 meV	< 10 meV	
Band structure (max η_{10})	< 20 meV	< 20 meV	
Equation of state (Δ -factor)	< 1 meV/atom (if possible)	smallest	

Please note that even for the SSSP Efficiency library we often made the conservative choice of choosing pseudopotentials with semi-core states in the valence; this greatly increases the cost of the calculations if many atoms of such elements are used, and might not be needed in bulk metallic solids.