Precision and efficiency in solid-state pseudopotential calculations

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Despite the enormous success and popularity of density-functional theory, systematic verification and validation studies are just starting to appear [1]. Here, we propose a protocol to test publicly available pseudopotential libraries, based on several independent criteria including verification against all-electron equations of state and plane-wave convergence tests for phonon frequencies, band structure, cohesive energy and pressure. Adopting these criteria we obtain curated pseudopotential libraries (named SSSP or standard solid-state pseudopotential libraries), that we target for high-throughput materials screening ("SSSP efficiency") and high-precision materials modelling ("SSSP precision").

References

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