EXTENDED NORM-CONSERRVING PSEUDOPOTENTIIALS

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The principles of generalized norm conservation [1] and systematic convergence optimization [2] have been combined to generate pseudopotentials of accuracy and efficiency competitive with augmented potentials.[3] These ONCVPSPs, consisting of a local potential and a diagonal non-local operator, can be based on valence plus shallow-core state or valence plus scattering-state all-electron wave functions for each angular momentum ℓ. This approach has been extended to allow deeper core levels to become active to enable simulations of materials at extreme temperatures and pressures. The original algorithms developed to construct ONCVPSPs have been modified and are now robust for as many as 5 non-local projectors per ℓ. Significantly higher plane-wave cutoffs are of course necessary. The new approach can also be used to extend accuracy to high-lying conduction bands by adding more scattering states to standard potentials. Dirac all-electron wave functions are used to construct ONCVPSPs simulating fully-relativistic calculations.

These extended norm-conserving potentials perform comparably to the standard variety in ambient-conditions benchmark tests. For extreme-condition testing, a confined-single-atom model was developed which compared well for pressure vs. volume and temperature with close-packed solid calculations up to Ts of ~5 Ha. This was then used to compare all-electron and pseudo confined atoms up to ~100 Ha and densities ~10 times ambient. Finally, close-contact forces needed for high-T AIMD simulations were tested, and found to remain accurate with a great deal of non-local projector overlap. Such AIMD simulations and comparisons of computed equations of state to experiment have yet to be performed.

References

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