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Optimized norm-conserving Hartree-Fock pseudopotentials[1]
ERIC J. WALTER, College of William and Mary, WISSAM A. AL-SAIDI, College of William and Mary — We report soft Hartree-Fock based pseudopotentials obtained using the optimized pseudopotential method [2]. The spurious long range tail due to the non locality of the exchange potential is removed using a self-consistent damping mechanism as employed in exact exchange [3] and recent Hartree-Fock pseudopotentials[4]. The binding energies of several dimers computed using these pseudopotentials within a planewave Hartree-Fock code show good agreement with all-electron results.

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