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Generation of soft pseudopotentials from and for correlated methods. MICHAEL BENNETT, CODY MELTON, North Carolina State Univ, LUKE SHULENBURGER, Sandia National Laboratories, LUBOS MITAS, North Carolina State Univ — We study several types of soft, semilocal pseudopotential constructions based on one-body and many-body approaches. The construction is formulated as an (inverse) optimization that can explore several types of optimization criteria, for example, matching one-particle properties such as orbital norm-conservation/shape-consistency, reproducing excitation energies in Hartree-Fock and correlated methods and matching correlated density matrices. It is known that, in general, this is an ill-conditioned problem where additional constraints need to be supplied to achieve converged results in a reasonably robust manner. The constructed effective operators are tested in high accuracy correlated calculations of atoms and small molecules. By a combination of methods we are able to obtain pseudopotentials for selected elements in the first two rows with accuracy that reproduce all-electron excitations and binding curves with 0.05-0.01 eV accuracy despite using only a very restricted number of gaussian terms in each L-channel. We therefore show that significant improvements in accuracy of pseudopotentials are feasible and therefore provide an opportunity for an overall increase in the accuracy and efficiency of QMC methods and other correlated approaches for valence-only calculations.

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