BASIS SETS IN CORRELATED EFFECTIVE POTENTIAL CALCULATIONS

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Due to the behavior of the pseudo-orbitals near nuclei, basis set selection in shape-consistent effective potential calculations can be problematic in studies using correlation techniques based on virtual orbital expansions (configuration interaction, etc.). In this work we quantify the magnitude of the problem and give simple rules for the selection of correlating functions in a manner that parallels the use of simple diffuse primitives in all-electron work. Our calculations show the problem to be substantial for s and p basis sets, but negligible for higher l. Computed s and p shell correlation energies, as determined in single and double promotion CI calculations, can be increased by 3% to 7%, as compared to basis sets using simple diffuse primitives for the systems tested.