RELATIVISTIC EFFECTIVE CORE POTENTIALS FROM ATOMIC NODELESS VALENCE SPINORS

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A relativistic effective core potential (RECP) method is enhanced to address problems due to nonlocal effects traceable to outer-core electrons. Atomic calculations using small-core RECPs explicitly treating outer core electrons form the basis for extracting two-component nodeless valence spinors (NVS) which are used to generate new large-core RECPs. Errors in published large-core RECPs are shown to result from the inherent arbitrariness in the choice of match points that define shape-consistent pseudospinors and thus lead to an improper representation of nonlocal effects. These are made salient via calculations on InH and InCl with an REP derived from NVSs. The bond lengths increase relative to those calculated with published large-core RECP and are in agreement with those obtained using a frozen 4d-subshell, small-core RECP for In.