RELATIVISTIC PSEUDOPOTENTIONAL INCORPORATING CORE/VALENCE POLARIZATION AND NON-LOCAL EFFECTS

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A relativistic pseudopotentional (RPP) for use in ab initio molecular electronic structure calculations is derived in the context of a pseudospinor-based relativistic effective core potential (RECP) method. The resulting atom-specific RPP has salient features of the RECP imbedded within it while retaining the form of a functional that is dynamically defined at runtime when used in calculations on atoms and molecules. The RPP is determined from Dirac-Fock wave functions for the isolated atom. The development of a pseudopotentional is shown to be necessary because of the inability of currently available RECPs to describe the outercore region of atoms properly and thus account for core/valence correlation effects in both atomic and molecular environments.