RELATIVISTIC PSEUDOPOTENTIONAL IN MOLECULAR ELECTRONIC STRUCTURE CALCULATIONS

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The incorporation of a nodeless-valence-spinor-based relativistic pseudopotentional (RPP) into ab initio molecular electronic structure calculations is presented. Outercore two-electron interactions are included in the RPP by means of coefficients that are self-consistently determined and are defined in the context of the final molecular wavefunction. This form permits polarization of outercore shells analogous to that occurring in all-electron non-correlated molecular calculations while retaining these shells as part of the atomic pseudopotentional. The RPP accounts for core/valence correlation effects when used in configuration interaction calculations.