AB INITIO RELATIVISTIC INNER-CORE/OUTER-CORE POTENTIAL METHODS IN ELECTRONIC-STRUCTURE CALCULATIONS

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Progress is reported in developing relativistic large-core potentials in which the outer core is treated especially flexibly so that it can relax and polarize in molecular environments (pseudopotentionals vs. pseudopotentials). The advantage is that more complicated treatment of the outer-core electrons is simpler and less costly than putting these electrons into the valence space.
Calculations on actinide molecules are reported at the self-consistent-field and spin-orbit-configuration-interaction levels using a one-electron basis of two-component spinors. Comparisons to the use of a one-component orbital basis are discussed.