MCDHF adjustment of relativistic pseudopotentials

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Pseudopotentials are used for simulating atomic cores and for implicitly incorporating relativistic effects in valence *ab initio* calculations. The energy-consistent pseudopotentials of the Stuttgart/ Dresden group are designed to reproduce atomic valence spectra derived from all-electron relativistic calculations. While we used scalar-relativistic Wood-Boring (WB) reference data in connection with WB or Dirac-Hartree-Fock (DHF) spin-orbit splittings for this purpose in the past, a recently introduced 'direct' determination of 2-component pseudopotentials in multi-configuration DHF calculations (including the Breit interaction and QED effects) should be particularly well suited for very heavy atoms. We present small-core pseudopotentials for post-d main-group elements (Ga - Tl, Ge - Pb, As - Bi) adjusted along these lines, and compare their performance, in atomic calculations and for properties of ground and excited molecular states, to results from all - electron calculations and to experimental data.