## On the Performance of No-Pair Ab Initio Model Potentials

Christel M. Marian, GMD-SCAI, St. Augustin
Frank Rakowitz, Theoretische Chemie, U Bonn

Spin-free relativistic no-pair *ab initio* core model potentials are presented for the transition elements Sc to Hg. Combined with a one-center no-pair spin-orbit mean-field approach, they represent an efficient and reliable tool to perform two-component calculations on heavy element containing compounds.
For the diatomic oxides VO, NbO, TaO, NiO, PdO, and PtO the performance of the spin-free model potentials have been tested extensively against corresponding all-electron results, both at the Hartree-Fock and the correlated level, and the requirements on valence and intermediate basis sets used to represent the exchange and no-pair operators have been investigated. Further, we shall compare all-electron and AIMP results of spin-orbit calculations on $PtCH_2+$.