Development of New Relativistic Model Core Potentials (spdsMCPs) for First-row Transition Metal Atoms and Their Applications

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Abstract: Heavy metal clusters are difficult to calculate because of the following reasons: many electrons, relativistic effect, and electron correlation. Normal all-electrons treatment is faced with these problems and we must treat many electrons including inactive core electrons in heavy elements. Furthermore, we must consider relativistic effects at the same time, resulting in high-cost calculations. However, we can overcome these problems by using so-called effective core potential (ECP) or model core potential (MCP).

For transition metal elements, we have developed two types of MCPs, *ds*MCP and *pds*MCP. Both MCPs have described well the ground state properties of transition-metal complexes. However, the MCPs have a weak point for describing the excited states: We have recently developed new relativistic model core potentials, spdsMCP, in which 3s, 3p, 3d and 4s electrons explicitly, for the first-row transition-metal atoms.

We demonstrated that the present spdsMCP basis sets have excellent performance in describing the electronic structures of atoms and molecules, bringing about accurate excitation energies for atoms and very good spectroscopic constants for some molecules, which aim at good performance for both the ground and excited states.

The first-low transition metal dimers are difficult to calculate in spite of their simple structures, because the dimers have different characteristic electron configurations for each ground state. Using the basis sets complete active space self-consistent field (CASSCF) with twelve active orbitals and second-order multiconfiguration quasidegenerate perturbation (MCQDPT2) theory were performed for the first-low transition metal dimers. Among these transition metal dimers, chemical bonding and magnetic interaction of Mn_2 are the most difficult to calculate and first examined Mn_2. Our spdsMCP gave excellent spectroscopy constants for Mn_2. The results of the other first-low transition metal dimers will show in congress.

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