Program and Abstracts

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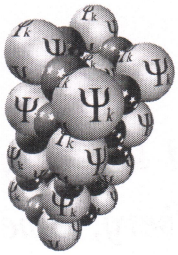

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Rational Design of Single Molecule Magnets – Density Functional Perspective

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Abstract

In recent years, there has been a growing interest in the single molecule magnets (SMM) that display a bistable (up/down) magnetic spin state below certain critical temperature because of their potential applications. Obtaining SMMs working at room temperature is reduced to understanding Zero-Field-Splitting (ZFS) parameters that determines the magnetic anisotropy of isolated transition metal complex. In this work, computational study of the magnetic anisotropy in series of transition metal complexes, when changing the metal ion, or the ligands, in a controlled way will be presented. In order to achieve this goal, ligand field DFT method (LF-DFT) [1] is applied for the calculations of ZFS parameters and analysis of magnetic anisotropy. LF-DFT works by evaluating DFT energies of all the Slater determinants arising from a d^n configuration of the transition-metal ion in the environment of coordinating ligands using Kohn-Sham orbitals. This set of energies is then analysed within a LF model to obtain variationally energies and wavefunctions of the ground and excited states. In doing so, both dynamical correlation (via exchange-correlation energy) and non-dynamical correlation (via LF CI) are considered. Spin-orbit coupling constant was deduced from the LF analysis of the energy splitting of the spinors, obtained by the ZORA spin-orbit DFT calculations. Finally, ZFS parameters were obtained using an effective Hamiltonian from the lowest eigenvalues and corresponding eigenvectors from LF-DFT multiplet calculations. With this methodology, we accurately predict magnitude, sign of the ZFS parameters, orientation of the principal magnetic axes, and we can pin-point the excitations that control magnetic anisotropy. In this way, we rationalize the connection between the electronic structure, excited states and magnetic properties of transition-metal complexes. The present strategy will be illustrated by discussion of the magnetic anisotropy in trigonal-bipyramidal complexes of Ni(II) [2], scorpionate complexes [3], and octahedral complexes of Mn(IV) [4].

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