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Rational design of single molecule magnets

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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, first, it was necessary to correctly determine the spin-ground state of transition metal ions, not straightforward task [1]. We performed detailed density functional based calculations probing the spin-state of these systems using variety of density functional approximations (DFAs). OPBE, SSB-D and S12g emerged to be one of the best DFAs for this task. In a second step, LF-DFT [2] is applied for the calculations of ZFS parameters. In addition to accurate prediction of magnitude, sign of the ZFS parameters, and orientation of the principal magnetic axes, we can pin-point the excitations that control magnetic anisotropy. In this way, we rationalize the connection between the structure, spin-ground state, excited states and magnetic properties of transition-metal complexes. The present approach will be illustrated by discussion of the magnetic anisotropy in trigonal-bipyramidal complexes of Ni(II) [3], scorpionate complexes [4], and octahedral complexes of Mn(IV) [5].

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[1] M. Swart, M. Gruden, *Acc. Chem. Res.*, **49**, 2690 (2016).

[2] M. Atanasov, C.A. Daul, C. Rauzy, *Chem. Phys. Lett.* **367**, 737 (2003). 367, 737.

[3] M. Gruden-Pavlović, M. Perić, M Zlatar, P. García-Fernández, *Chem. Sci.* **5**, 1453 (2014).

[4] M. Perić, A. García-Fuente, M. Zlatar, C. Daul, S. Stepanović, P. García-Fernández, M. Gruden-Pavlović, *Chem. -Eur. J.* **21**, 3716 (2015).

[5] M. Zlatar, M. Gruden, O. Y. Vassilyeva, E. A. Buvaylo, A. N. Ponomarev, S. A. Zvyagin, J. Wosnitza, J. Krzystek, P. García-Fernández, C. Duboc, *Inorg. Chem.* **55**, 1192 (2016).