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Exploring magnetic properties of single molecular magnets

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Prominent physical properties of a broad family of single-molecule magnets based on the transition metal ions with the unfilled electronic 3d-orbital shell are characterized and their potential for practical applications is revealed. In particular, molecular magnets can serve as elements of magnetic memory, quantum bits and molecular refrigerants [1].
To relate the observable characteristic of single-molecule magnets with their internal electronic structure and magnetic anisotropy, the multi-electron wave functions should be calculated by solving Schrodinger equation for a general all-electron Hamiltonian of the system. This is done for mononuclear complexes such as metal-organic molecule, based on explicitly correlated (multiconfigurational) ab initio quantum chemical calculations performed with the use of Firefly computer program [2].
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[2] M.W.Schmidt, K.K.Baldridge, J.A.Boatz, S.T.Elbert, M.S.Gordon, J.H.Jensen, S.Koseki, N.Matsunaga, K.A.Nguyen, S.Su, T.L.Windus, M.Dupuis, J.A.Montgomery. J.Comput.Chem. 14, 1347-1363 (1993).

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