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Excited spin multiplets of magnetic molecules from a DFT-based many-spin Hamiltonian KYUNGWHA PARK, Georgetown Univ., Naval Research Lab, and Howard Univ., MARK PEDERSON, C. STEPHEN HELLBERG, Naval Research Lab, Washington DC — It has been recently demonstrated within spin-polarized density-functional theory that the electronic structure and magnetic properties of large magnetic molecules consisting of up to 200 atoms can be calculated and that the calculated ground-state properties agree well with experiment. However, the excited spin multiplets of magnetic molecules, due to strongly coupled metal ions, are not well understood especially for the case with large magnetic anisotropy. In this talk, we address the necessity of using a many-spin Hamiltonian to explore the excited spin multiplets and present our method to model the Hamiltonian for an isolated Mn_{12}-acetate molecule using spin-polarized density-functional theory. We identify the total magnetic moments of low-lying excited spin multiplets by diagonalizing the model Hamiltonian (dimension of $10^8 \times 10^8$). We also show our calculated energy gaps between the excited and the ground spin multiplets and predict magnetic anisotropy barriers of the spin multiplets. Finally, we compare our results with experimental data.

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