Charge Transfer in Single-Molecule Magnetic Complexes $[Mn_{12}O_{12}(O_2CR)_{16}(H_2O)_4]$

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Single-molecule magnetic (SMM) complexes $[Mn_{12}O_{12}(O_2CR)_{16}(H_2O)_4]$, with R=-H, $-CH_3$, $CHCl_2$, $-C_6H_5$, have twelve Mn atoms in the core, eight of them are in 3+ charge state and located at peripheral ring of the molecule, while the four remaining Mn atoms in the center of the molecule are in 4+ charge state. When the SMM molecule is receiving the additional electron by excitation, this electron is localizing on one of the peripheral Mn atom, and the charge state of this atom is changing from Mn^{3+} to Mn^{2+}, what is confirmed by experiment measuring the Mn-O bond lengths [Inorg. Chem. 2017, 56, 10706]. In order to develop the SMM with high catalytic activity, it is very important to know the energy barrier for electron transfer from Mn^{2+} atom to another Mn^{3+} atom located on diametral site of the molecule, in order to stimulate oxidation reaction. We are calculated the minimum energy pathway for electron transfer in tunneling regime calculating the energy barrier for electron motion by plotting the profile of electrostatic potential along possible pathways.

Acknowledgements
US Department of Energy Basic Energy Sciences Energy Frontier Research Centers under Grant No. DE-SC0019330