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Spin-state energetics of Fe complexes from an optimally-tuned range-separated hybrid functional GEORGIA PROKOPIOU, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel — We assess whether the optimally-tuned range separated hybrid (OT-RSH) functional approach can predict the correct ground-state electronic configuration and spin-state energetics of complexes that can potentially exhibit multiple spin configurations. To that end, we investigate eight iron complexes: Four spin-crossover complexes, for which reference data from other approximate density functionals are available, and four smaller complexes, for which reference *ab initio* data are available.

We show that the spin-state energetics are mostly governed by the percentage of short-range exact exchange and are only weakly influenced by the choice of range-separation parameter. However, the electronic structure, especially the HOMO-LUMO gap, is much more sensitive to the range-separation parameter. We find that use of OT-RSH improves the electronic structure, as compared with that obtained from semi-local or global hybrid density functionals. However, as with global hybrid functionals, correct prediction of the ground-state in the spin-crossover compounds requires a reduction in the amount of short-range exact exchange, possibly owing to a larger role of static correlation.

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