MODELING LASER-INDUCED SPIN CROSSOVER TRANSITIONS USING TIME-DEPENDENT DENSITY FUNCTIONAL THEORY

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The light-induced magnetic bistability of square pyramidal and octahedral Ni(II) macrocyclic ligand complexes have been investigated using density functional theory (DFT) and linear response time-dependent DFT (TD-DFT) methods considering the MN12-SX exchange-correlation functional and the def2-TZVP basis set. The stability of the light–mediated reversible ligand coordination and the switching of magnetic properties have been characterized by identifying the active electronic excited states both in singlet and triplet spin configuration involved in the light-induced excited spin-state trapping. A Python code for localizing the intersystem crossing points between singlet and triplet spin states is presented and characteristics of these geometry structures as well as spin couplings are discussed.