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Double-Exchange Model for Molecule-Based Magnets SERKAN ERDIN, MICHEL VAN VEENENDAAL, Department of Physics, Northern Illinois University, DeKalp, IL and Advanced Photon Source, Argonne National Laboratory, Argonne, IL — We report a detailed study of a model proposed for the molecule-based magnets, which is similar to the double-exchange mechanism. The model is applied to a two-dimensional periodic complex made of a transition metal and an organic molecule in which the electronic structure is described by effective d orbitals of the transition metal ion at infinite Hund's coupling limit and the lowest unoccupied molecular orbital of the organic molecule. Depending on the average electron density of the organic molecules and various superexchange couplings between metal ions' core spins, magnetic states of the complex are investigated. In Monte-Carlo calculations for a model Hamiltonian, as a function of electron density on the organic molecule, the average magnetization and critical magnetic ordering temperatures are determined.

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