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Determination of High-Spin to Low-Spin Phase Transition of Organic Spintronic Device by Monte Carlo Simulation of 3D Ising-like Model ASHLEY S. DALE, AARON MOSEY, Indiana University - Purdue University Indianapolis, P. A. DOWBEN, University of Nebraska, HORIA PETRACHE, RUIHUA CHENG, Indiana University - Purdue University Indianapolis — Spin crossover (SCO) materials are a possible solution to challenges faced in developing new nonvolatile voltage-controlled micro and nanoelectric devices. The design and implementation of devices benefits from ab initio calculations determining device characteristics and behaviors. Previous work by Bousseksou et al. shows that the phase transition between the high-spin (HS) and low-spin (LS) states of a SCO material may be described by a 2D Ising-type model, where the Ising "spin-up" and "spin-down" states correspond to the HS and LS states respectively. 2D Ising-type models have successfully captured the behavior of 2D thin films such as graphene and CrSiTe, and 2D Monte Carlo Ising Model simulations already provide insight into the switching mechanism for experimentally observed thin film behaviors. By expanding the established 2D model to a 3D model for thin-film heterostructures, we capture the behavior of a SCO-based device by simulating the phase transition of a Fe(II) ion centered octahedral coordination compound adsorbed to a ferroelectric polymer in the presence of temperature change and electric field excitation. Furthermore, by varying parameters in the Ising-like Hamiltonian for the SCO molecules, we better direct the choice of potential SCO molecular candidates for viable spintronic device designs.

Ashley Dale
Indiana University - Purdue University Indianapolis

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