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Density Functional Plus Dynamical Mean Field Study of Spin Crossover Molecule JIA CHEN, Departemtn of Applied Physics and Applied Math, Columbia University, ANDREW MILLIS, Departemtn of Physics, Columbia University, CHRIS MARIANETTI, Departemtn of Applied Physics and Applied Math, Columbia University — We report a density functional plus dynamical mean field study of spin crossover molecule Fe(phen)2(NCS)2. The temperature dependent magnetic susceptibility, Fe-d spectral and total energy were calculated and compared with experimental magnetization, metal L-edge x-ray adsorption spectroscopy. The importance of dynamic effect on energetics is demonstrated by comparison with density functional plus U method, and the role of full charge self-consistency is identified. Moreover, the local spin density plus U (LSDA+U) method with exchange interaction explicitly included is shown to dramatically overemphasize magnetic interaction.

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