Moments in Materials Presentation:

Extending dynamical mean-field theory to chemical systems: a study of spin-crossover molecule

Speaker: Jia Chen
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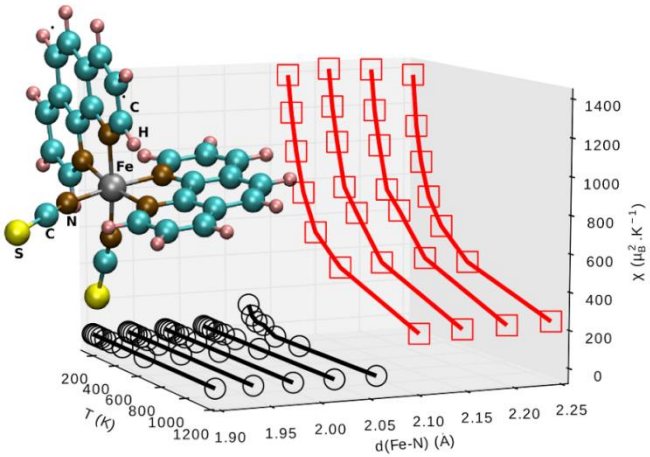
Strongly correlated materials can exhibit a wide range of interesting properties. However, understanding and predicting behaviours of these materials is very challenging from a theoretical standpoint. As the state of the art theoretical method for strongly-correlated systems, dynamical mean-field theory (DMFT) has provided us insight on various materials and phenomena. Recently, promising progress has been made in generalizing DMFT to chemical systems. Utilizing DMFT as electronic structure calculation method, we studied a spin-crossover molecule: $Fe(phen)_2(NCS)_2$. In general, good correlation between theory and experiments were achieved for measurables including magnetic susceptibility, x-ray adsorption spectroscopy, and total energy. The metal-to-ligand bond length was identified as the control parameter for spin state.



Selected references
G. Kotliar and D. Vollhardt, Phys. Today 57(3) 53 (2004)
N. Lin, C. A. Marianetti, A. J. Millis and D. R. Reichman. Phys. Rev. Lett 106 096402 (2011)