

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Magneto-electric multiferroic behavior in a metal-organic framework VIVIEN S. ZAPF, National High Magnetic Field Lab, Los Alamos National Lab, Los Alamos, NM, PINAKI SENGUPTA, Nanyang Technological University, Singapore, CRISTIAN BATISTA, Theoretical Division, Los Alamos National Lab, FARZANA NASREEN, NHMFL, LANL and New Mexico State University, FREDERIK WOLFF-FABRIS, NHMFL, LANL, now at Dresden Hochfeld Labor, ARMANDO PADUAN-FILHO, Universidade de Sao Paulo — We will discuss strong magneto-electric coupling in the metal-organic compound $\text{NiCl}_2\cdot 4\text{SC}(\text{NH}_2)_2$ (also known as a metal-organic framework or molecular magnet). Magneto-electric multiferroic behavior is traditionally investigated in transition-metal oxides, however we are expanding the field to metal-organics, which are designable materials with soft lattices and electrically polar organic elements. In this material we observe a magnetic field-induced change in the electric polarization of $50 \mu\text{C}/\text{m}^2$ driven by ordering of the Ni $S = 1$ spins. We can model it in terms of a combination of exchange striction and crystal electric fields, and Quantum Monte Carlo simulations of these effects provide an excellent fit to the data. We find that the induced electric polarization is a sum of $\langle S_z^2 \rangle$ and the nearest neighbor correlation function $\langle S_i \cdot S_j \rangle$. The presence of electrically polar thiourea molecules $[\text{SC}(\text{NH}_2)_2]$ amplifies the effect of small magnetically induced crystal distortions on the electric polarization.

Vivien S. Zapf
National High Magnetic Field Lab,
Los Alamos National Lab, Los Alamos, NM

Date submitted: 13 Dec 2010

Electronic form version 1.4