

Project Title:

Monte Carlo simulations for organic multiferroic systems

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Multiferroics refers to coexistence of orders of different nature. In particular, the combination of magnetism and ferroelectricity has been the most extensively studied branch because of its potential for energy-efficient devices. In 2012, we published a theoretical paper on a new mechanism of multiferroics and magnetoelectric effects, arising from virtual fluctuations of electrons in frustrated Mott insulators [YK and C. D. Batista, Phys. Rev. Lett. 108, 097202 (2012)]. Our theory assumes a lattice structure comprising trimers of spin-1/2 magnetic moments. Recently, our collaborator succeeded in synthesizing an organic compound that has such trimers as its building block, and the purpose of our numerical work is to refine our theoretical calculation to be compared with this new compound.

We derived an effective low-energy model by treating the weak interactions between spins on different trimers as perturbations. The resulting model is a variant of the Kugel-Khomskii Hamiltonian, combining magnetic and “orbital” degrees of freedom, both of which are represented by pseudospin-1/2 operators. The main purpose of this numerical work is to map out the phase diagram for classical ground states, by replacing the pseudospin-1/2 operators with classical vector spins. Our method is the classical Monte Carlo simulation on such an effective classical spin-orbital model.

The calculation is still under way by the time this report is submitted, but we have already obtained quite a few interesting results (to be published). We confirmed that the magnetization curve, the longitudinal spin susceptibility, and also the

dielectric constant reproduce nicely the experimental observation in the organic multiferroic material mentioned above. In addition, our simulations predicted a sequence of fractional magnetization plateaux at low temperature, which is well below the experimental base temperature. It will be very interesting to see if such an exotic feature is realized in this material, which could be one of the potential new directions of this project.