Crystallographic Description of Ordered Toroidal Moments

S Gnewuch[1], E Rodriguez[2]
[1]University of Maryland, College Park, Maryland, MD, [2]University of Maryland
sgnewuch@umd.edu

The symmetry of a quantum material system enables us to understand and predict the system's properties under different thermodynamic conditions. This is particularly true in ferroic systems, which are classified by the broken symmetry across their temperature-dependent phase transitions. For example, above the transition temperature of a ferromagnet under no applied field, the magnetic moments are randomly oriented in a paramagnetic state. Below the transition temperature, the moments align along a crystallographic direction, breaking time-inversion symmetry. In addition to the three well-studied classes of ferroics (ferromagnets, ferroelectrics, and ferroelastic) we are studying materials expected to exhibit ordering according to a fourth category, known as ferrotoroidics. As a ferrotoroidic material is cooled below its ordering temperature into a magnetically ordered state, the toroidal moments align along a crystallographic direction, breaking space-time inversion symmetry. Candidate ferrotoroidic materials are proposed based upon their magnetic point group symmetry and magnetoelectric properties [1]. The most well-studied candidate material is $LiCoPO_4$. Notably, Zimmerman and Fiebig *et al.* performed second harmonic generation experiments on $LiCoPO_4$ under magnetic and electric fields and observed a hysteretic response characteristic of ferroics [2]. There are several structural analogs to $LiCoPO_4$, including $LiFePO_4$ which exhibits the same magnetic structure as $LiCoPO_4$ (*Pnma'*), as well as $LiMnPO_4$ whose magnetic structure would not permit ferrotoroidal order (*Pn'm'a'*). Two years ago at this conference, I presented results of neutron diffraction studies on solid solutions between these end members $LiMn_xCo_{1-x}PO_4$ and $LiMn_xFe_{1-x}PO_4$. For all the studied members, they exhibited the same magnetic space group symmetry as $LiCoPO_4$, which is evidence that this series of materials can be considered tunable ferrotoroidic candidates. In the following year I developed this idea further, extending the model for ordered toroidal moments proposed by Ederer and Spaldin [3] to these series as well as other candidate materials. The purpose of this presentation is discuss how to not only model a ferrotoroidic state, but also a paratoroidic, antiferrotoroidic, and nonferrotoridic system according to crystallographic conventions. [1] Gnewuch, S.; Rodriguez, E.E. *J. Solid State Chem.* **2019**, *271*, 175 - 190. [2] Zimmerman, A. *et al. Nature Comm.* **2014**, *5*, 4796. [3] Ederer, C.; Spaldin, N. A. *Phys. Rev. B* **2007**, *76*, 214404. Acknowledgements: The authors gratefully acknowledge funding from the U.S. DOE Office of Science (Grant#: DE-SC0016434).