MAR08-2007-000848

Abstract for an Invited Paper
for the MAR08 Meeting of
the American Physical Society

Towards a microscopic theory of toroidal moments in periodic crystals[1]

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The recent resurgence of interest in magnetoelectric multiferroics has prompted discussion of the relevance of the concept of magnetic toroidal moments in such systems. In particular, the toroidal moment has the same symmetry as the antisymmetric part of the linear magnetoelectric tensor, suggesting a role in mediating coupling between magnetization and electric polarization in multiferroics. In addition, materials in which the toroidal moments are aligned cooperatively – so-called ferrotoroidics – have been proposed to complete the group of primary ferroics[2]. Here we review the basic microscopic and macroscopic definitions of toroidal moments and illustrate the difficulties in evaluating the toroidal moment of an infinite periodic system. We show that periodic boundary conditions give rise to a multivaluedness of the toroidal moment per unit cell, in close analogy to the case of the electric polarization in bulk periodic crystals. We then evaluate the toroidal moments of several multiferroic and magnetoelectric materials ($BaNiF_4$, $LiCoPO_4$, $GaFeO_3$ and $BiFeO_3$) in the "localized dipole limit", where the toroidal moment is caused by a time- and space-reversal symmetry-breaking arrangement of localized magnetic moments[3].

[1]In collaboration with Claude Ederer, Trinity College, Dublin

[2]B.B. Van Aken, J.P. Rivera, H. Schmid and M. Fiebig, Nature 449, 702 (2007).

[3]C. Ederer and N.A. Spaldin, arXiv:0706.1974v1 [cond-mat.str.el], Phys. Rev. B in press.