Parity odd magnetism in transition metal oxides

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The formation of parity and time reversal odd magnetic order accompanies the breaking of time and space inversion symmetry in materials. Here we discuss different representatives of this ordering including magnetic hedgehogs, toroidal and magnetic quadrupole moments. We further present a scheme to calculate these multipole moments within the framework of first-principles calculations[1]. By applying our approach on two different CuO materials we finally explore different scenarios for the appearance of this order.

In CuO experimental measurements by resonant x-ray diffraction revealed an antiferro-toroidal order[2] in the low temperature antiferromagnetic phase. Our calculations show that these moments originate from a strong hybridization between Cu-dx^2-y^2 orbitals with neighboring O-*p* orbitals. This interaction enforces a spin asymmetry around Cu, which creates toroidal moments.

In contrast in our second example, $HgBa_2CuO_4$, the multipolar order inferred from neutron measurements[3] originate from a ''dynamic'' scenario. Here the coupling of spin and phononic system creates a quasi-static multipolar order in absence of static magnetic ordering. Finally we discuss the implications of such dynamic ordering for other materials.

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[2] V. Scagnoli, U. Staub, Y. Bodenthin, R. A. de Souza, M. Garcia-Fernandez, M. Garganourakis, A. T. Boothroyd, D. Prabhakaran, and S. W. Lovesey, Science **332**, 696 (2011).

[3] S. W. Lovesey and D. D. Khalyavin, arXiv **cond-mat.str-el**, (2015).