Poster

Anti-magnetoelectricity, a hidden order probed by Dynamical Magnetic Charges

M. Braun[1,2], B. Guster[1], A. Urru[3], H. Kabbour[2], E. Bousquet[1]

[1]Physique Théorique des Matériaux, QMAT, CESAM, Université de Liège, B-4000 Sart-Tilman, Belgium

[2] Unité de Catalyse et Chimie du Solide, UCCS CNRS, Centrale Lille, ENSCL, Université de Lille, F-59000 Lille, France

[3] Department of Physics and Astronomy School of Arts and Sciences Rutgers, The State University of New Jersey, USA

Maxime.braun@uliege.be

Magnetoelectric materials, capable of manifesting a coupling between magnetic and electric properties at the static level, may offer the potential for manipulating one through the other via the application of external magnetic or electric fields. This coupling is symmetry dependent, with the analysis of the material's magnetic space group providing insight into how the coupling will manifest under varying conditions. However, in some cases, the absence of a response from the bulk may occur due to the cancelation of local responses, known as the dynamical magnetic charge (DMC). Those DMC relate the induced magnetization from an atomic displacement, i.e. an analogue to the Born effective charge (BEC) relating the polarisation induced by an atom displacement. This lack of coupling due to cancellation effects renders the material "antimagnetoelectric [1]", akin to the hidden order explained in antiferromagnetics since Neel's discovery. This phenomenon can be identified from material's specific space group. Indeed, the Wyckoff positions, coupled with their magnetic point group symmetry, elucidates the geometric arrangement of the DMC matrix, mirroring the magnetoelectric tensor (α_{ij}) characteristics within this particular point group.

Our research utilizes an ab initio approach to computationally investigate the electronic and lattice mediated response that define anti- magnetoelectric behaviour. Specifically, we calculate the BECs and the DMCs, which are further employed to evaluate the linear and non-linear magnetoelectric tensor [2-3], of the materials under study. We apply those calculations and symmetry analysis in the multiferroic material $BiCoO_3$, which shows typical anti-magnetoelectric properties with huge local atomic responses that perfectly cancel out within all the polar displacements of the infrared active modes. We also found that the DMCs in $BiCoO_3$ are large from both spin (S) and orbital (L) origins.

Given the challenges in experimentally verifying these computationally predicted properties, we propose the adoption of novel experimental techniques such of high-energy electron beams [4] with sufficient wavevector magnitude to probe zone-boundary phonon modes. These techniques could validate the presence of DMCs in operational environments, thereby opening new pathways for the exploration of (anti-)magnetoelectric materials.

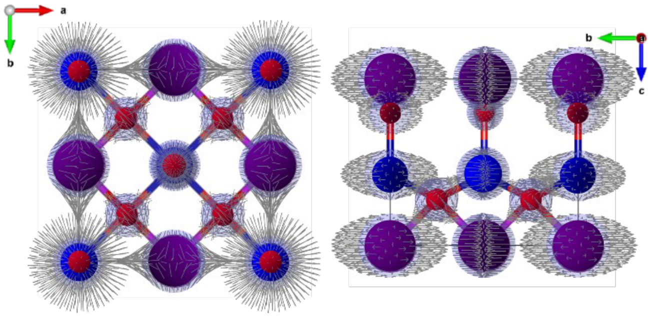

Fig 1. $BiCoO_3$ (Bismuth in purple, Cobalt in blue and Oxygen in red) structure with grey arrow representing the magnetization induced by displacing the atom by r which is directly proportional to the atomic DMC.

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