

Theory of Condensed Matter: Hard Condensed Matter

Nov. 22, 2017 at 3 p.m.
ComZone 01-620 (Staudinger Weg 7)

Eric Bousquet
Université de Liège

Magnetoelectric response from first- principles: microscopic understanding and design rules

First-principles calculations based on density functional theory (DFT) appeared to be valuable tools to compute the strength of the magnetoelectric response of materials and to understand its microscopic origin. The methods are becoming sufficiently reliable and predictive to be used in the search for new magnetoelectric materials.

In this talk I will present the state of the art of the different first-principles techniques that can be used to compute the magnetoelectric response of a crystal under electric or magnetic fields. I will show their applications on several systems such as the prototypical magnetoelectric material Cr_2O_3 , LiFePO_4 and the troilite phase of FeS . For each of these systems, I will discuss the different microscopic mechanisms that drive their response: electronic versus lattice mediated and spin versus orbital origins. Then, I will present two original examples of strain engineered ferroelectric and magnetoelectric responses in initially “non-functional” materials: CaMnO_3 and NaMnF_3 . I will also profit the occasion to introduce some related and exotic features of magnetoelectricity: magnetoelectric monopoles and (ferro)toroidal moments.