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First-principles calculation of the full orbital magnetoelectric response ANDREI MALASHEVICH, UC Berkeley, IVO SOUZA, Centro de Fisica de Materiales, San Sebastian, SINISA COH, DAVID VANDERBILT, Rutgers University — The possibility of a quantized magnetoelectric (ME) effect in Z_2 topological insulators suggests that the orbital part of the ME response can, at least in principle, be comparable in magnitude to the total response of known ME materials.[1] A band theory of the orbital ME response of generic insulators was recently developed,[2] paving the way for first-principles calculations. Two types of terms contribute to the response. The Chern-Simons term, which only depends on the unperturbed valence Bloch states, was the subject of a recent Wannier-based calculation.[1] The Kubo terms require a knowledge of the Bloch states at first order in the electric field and can be calculated by finite differences from the change in orbital magnetization induced by small electric fields.[2] We present preliminary results of such a calculation for Cr_2O_3, using the Berry-phase approach to calculate the electronic structure under a finite electrical bias. By monitoring the field-induced changes in orbital and spin magnetization and comparing the results obtained with and without structural relaxation, all contributions to the ME coupling can be computed.

[1]S. Coh *et al.*, arXiv:1010.6071.
[2]A. Malashevich *et al.*, New J. Phys. **12**, 053032 (2010)

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