First-principles study of the dynamical magnetic charge tensor

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Magnetoelectric (ME) materials are of fundamental interest and are investigated for their broad potential for technological applications. The search for, and eventually the theoretical design of, materials with large ME couplings present challenging issues. First-principles methods have only recently been developed to calculate the full ME response tensor α including both electronic and ionic (i.e., lattice-mediated) contributions.[1] In several materials, the dominant contribution to the ME response has been shown to be the ionic term $\alpha_{\rm ion}$, which is proportional to both the Born dynamical electric charge $Z^{\rm e}$ and its analogue, the dynamical magnetic charge $Z^{\rm m}$.[2] The dynamical magnetic charge also has contribution to other magnetic properties, e.g. piezomagntism and magnetic susceptibility. Here we present a theoretical study whose ultimate goal is to understand the mechanisms that would enhance the magnetic charge $Z^{\rm m}$. Using first-principles density-functional methods within a relativistic framework with the inclusion of the spin-orbit interaction, we calculate the atomic magnetic charge tensors $Z^{\rm m}$ for both Cr and O atoms in Cr_2O_3, and discuss how these contribute to the ME response and other magnetic properties in this material.

[1] A. Malashevich et al., Phys. Rev. B, **86**, 094430 (2012).
[2] J. Íñiguez, Phys. Rev. Lett. **101**, 117201 (2008).