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Calculating Magnetoelectric Susceptibilities from First Principles with an Applied Magnetic Field KRIS DELANEY, Materials Research Laboratory, UC Santa Barbara, NICOLA SPALDIN, Materials Department, UC Santa Barbara — First-principles methods are emerging as a valuable tool in the search for materials with strong magnetoelectric couplings. Here, we present a convenient route to computing magnetoelectric responses based on the introduction of a Zeeman response to an applied magnetic field. Prior successful approaches for computing the magnetoelectric response were largely based on the non-self-consistent application of an electric field to determine the field-induced distortion of the lattice from the effective charges of polar lattice modes. Subsequently, the electric-field-induced magnetization was computed, leading to the lattice-mediated part of the magnetoelectric response. In contrast, our approach in principle contains both the electric and lattice-mediated parts of the magnetoelectric response, and provides a more efficient method than the non-self-consistent application of an electric field. We compare both approaches using the example of Cr_2O_3, the prototypical magnetoelectric material.

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