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Longitudinal magnetoelectric susceptibility of Cr2O3: First-principles calculations using the converse approach SAI MU, A. L. WYSOCKI, K.D. BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska-Lincoln — Temperature-dependent longitudinal magnetoelectric (ME) susceptibility of Cr2O3 is calculated as a response of the magnetization M to the applied electric field E. The ionic displacements are found using the calculated force constant matrix and Born effective charges. The exchange parameters are calculated using total energy calculations for different spin configurations on the perturbed lattice, and the magnetization is evaluated using the pair cluster approximation to the quantum spin-3/2 Hamiltonian. When similar approximations are used, the results agree with the inverse approach of Mostovoy et al. [Phys. Rev. Lett. 105, 087202 (2010)]. The electronic contribution is found to be approximately 40% of the ionic contribution and opposite in sign to it. The ME susceptibility is found to depend strongly on the choice of the Hubbard U parameter, increasing as U is increased. On the other hand, the ME response is only weakly depressed by the inclusion of intersite spin correlations within the pair cluster approximation. The methodology developed here can facilitate the search for new materials with desirable ME properties.

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