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First-Principles Study of Large Magnetoelectric Coupling in Triangular Lattices KRIS T. DELANEY, Materials Research Laboratory, UC Santa Barbara, MAXIM MOSTOVOY, Zernike Institute for Advanced Materials, University of Groningen, The Netherlands, NICOLA A. SPALDIN, Materials Department, UC Santa Barbara — We investigate, using density functional theory, the magnetoelectric coupling in a frustrated antiferromagnet in which the combination of frustration with magnetic interactions mediated by Anderson superexchange leads to a unconventional and large coupling between polarization and magnetic order. The nature of the superexchange mechanism can be manipulated through induced polarization of the lattice upon application of an electric field, leading to a strong magnetoelectric effect. We demonstrate the effect in a Mn-based triangular lattice that is closely related to the Kagomé structure, with modifications to avoid self-compensation of the induced magnetic order. For our study, we employ the VASP software package with LSDA+U for describing electron exchange and correlation effects. A fully noncollinear treatment of the spinors is essential to describe the complex spin structures that the system adopts.

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