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First-principles studies of dilute magnetic ferroelectrics LEIGH WESTON, School of Physics, The University of Sydney, Sydney, NSW 2006, Australia, XIANGYUAN CUI, SIMON P. RINGER, Australian Centre for Microscopy and Microanalysis, The University of Sydney, Sydney, NSW 2006, Australia, CATHERINE STAMPFL, School of Physics, The University of Sydney, Sydney, NSW 2006, Australia — Using first-principles density functional calculations, we have investigated the magnetic properties of dilute magnetic ferroelectrics (DMF), where a nominally non-magnetic ferroelectric host is doped with a small concentration of magnetic impurities. We find that DMFs may exhibit simultaneous electrical and magnetic polarization, consistent with recent experimental observations. A possible mechanism for magnetoelectric coupling was explored, and it was found that through a strong spin-lattice coupling, electric field induced switching of magnetization may be possible. Thus, DMFs may provide a route to achieving a single phase, room temperature multiferroic with strong magnetoelectric coupling.

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