

Abstract Submitted
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Properties of diluted antiferromagnets from atomistic simulations¹ SERGEY PROSANDEEV, LAURENT BELLAICHE, Physics Department, University of Arkansas, Fayetteville 72701 — An effective Hamiltonian technique is used to study the effect of substituting Fe ions by non-magnetic elements (in a specific sublattice) on the properties of the (mostly) antiferromagnetic BiFeO₃ multiferroic material. Interestingly, for small concentrations of the non-magnetic element and at low temperature, this substitution creates a net magnetic moment (per volume), \mathbf{M} , that is directed along the antiferromagnetic moment \mathbf{L} (unlike in pure BiFeO₃), and that increases in size with the non-magnetic concentration. On the other hand, above a percolation threshold, the net magnetic moment diminishes in magnitude with the non-magnetic concentration while the magnetoelectric coupling is dramatically enhanced. The origin of these unexpected phenomena are discussed in detail. In particular, it is proposed that the enhancement of the magnetoelectric coupling is mostly due to an increase of the magnetic susceptibility.

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