

Abstract Submitted
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Prediction of electromagnons in BiFeO_3 from atomistic simulations¹ BRAJESH MANI, CHUN-MIN CHANG, SERGEY LISENKOV, INNA PONOMAREVA, Department of Physics, University of South Florida, Tampa, Florida 33620, USA — We developed a first-principles-based computational approach to study the finite-temperature complex dynamics in multiferroics. Application of this technique to one of the most well-known multiferroic, BiFeO_3 , revealed that the most general form of the magnetoelectric coupling that is allowed in any multiferroic, may produce an electromagnon in antiferromagnetic ferroelectric. Such an electromagnon shares most of the features with the magnon, but is activated by an electric, rather than magnetic, field. We also found that the A_1 phonon mode is repelled by the magnon mode, while the E phonon modes is rather insensitive to the presence of (electro)magnons. We believe that our findings will aid to a deeper understanding of electromagnon modes and their origin in multiferroics as well as provide a computational methodology for further research.

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