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Title:Atomistic molecular dynamic simulations of multiferroics
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Abstract:A first-principles-based approach is developed to simulate dynamical properties, including complex permittivity and permeability in the GHz-THz range, of multiferroics at finite temperatures. It includes both structural degrees of freedom and magnetic moments as dynamic variables in Newtonian and Landau-Lifshitz-Gilbert (LLG) equations within molecular dynamics, respectively, with the couplings between these variables being incorporated. The use of a damping coefficient and of the fluctuation field in the LLG equations is required to obtain equilibrated magnetic properties at any temperature. No electromagnon is found in the spin-canted structure of BiFeO<inf>3</inf>. On the other hand, two magnons with very different frequencies are predicted via the use of this method. The smallest-in-frequency magnon corresponds to oscillations of the weak ferromagnetic vector in the basal plane being perpendicular to the polarization while the second magnon corresponds to magnetic dipoles going in and out of this basal plane. The large value of the frequency of this second magnon is caused by static couplings between magnetic dipoles with electric dipoles and oxygen octahedra tiltings. © 2012 American Physical Society.
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Main heading:Magnetic couplings
Controlled terms:Computer simulation - Magnetic moments - Magnetic properties - Molecular dynamics
Uncontrolled terms:Atomistic molecular dynamics - Basal planes - Complex permittivity - Damping coefficients - Different frequency - Dynamic variables - Dynamical properties - Electric

dipole - Finite temperatures - Fluctuation fields - Landau-Lifshitz-Gilbert equations - LLG equation - Magnetic dipole - Multiferroics - Newtonians - Oxygen octahedra - Spin-canted structure - Static couplings - Two-magnons
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