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Dynamical couplings in ferroelectrics and multiferroics
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First-principle-based molecular dynamics simulations are developed and used to investigate dynamical phenomena in the Pb(Zr,Ti)O$_3$ (PZT) ferroelectric solid solutions and in the multiferroic BiFeO$_3$ system$^{2,3}$. Several interesting effects are reported, including: (1) the existence of two $E$ modes in PZT in the 50–75 cm$^{-1}$ range for temperatures smaller than $\simeq 200$ K when the system is in its $R3c$ phase. Such existence originates from a linear coupling between ferroelectric (FE) motions and tiltings of oxygen octahedra; (2) a Fermi resonance (FR) emerging from a nonlinear coupling between FE distortions and oxygen octahedra tilts. This FR manifests itself as the doubling of a nominally-single FE mode in a purely FE phase, when the resonant frequency of the FE mode is close to the first overtone of the oxygen octahedra tiltings; and (3) the prediction of an electromagnon peak, that results from specific interactions between magnetic dipoles, FE motions and oxygen octahedra tiltings, in BiFeO$_3$. Some of these results have been confirmed by recent Raman scattering experiments, and analytical models are also developed to better understand such effects.$^4$

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