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Dynamical couplings in ferroelectrics and multiferroics[1]

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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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[2]D. Wang, J. Weerasinghe,and L. Bellaiche, Phys. Rev. B **83**,020301(R) (2011).

[3]D. Wang, E. Buixaderas, J. Íñiguez, J. Weerasinghe,H. Wang, and L. Bellaiche,Phys. Rev. Lett. **107**, 175502 (2011).

[4]This work is done in collaboration with L. Bellaiche (University of Arkansas), J. Hlinka (Institute of Physics, Czech Republic), E. Buxiaderas (Institute of Physics, Czech Republic), J. Íñiguez (Institut de Ciència de Materials de Barcelona, Spain) and J. Weerasinghe (University of Arkansas)