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“Forbidden” phonon in the iron chalcogenide series¹ DAVID M. FOBES, IGOR A. ZALIZNYAK, ZHIJUN XU, GENDA GU, JOHN M. TRANQUADA, CMPMSD, Brookhaven National Lab, Upton, NY 11973-5000, USA — Recently, we uncovered evidence for the formation of a bond-order wave (BOW) leading to ferro-orbital order at low temperature, acting to stabilize the bicollinear AFM order, in the iron-rich parent compound, Fe_{1+y}Te [D. Fobes *et al.*, Phys. Rev. Lett. 112, 187202 (2014)]. Investigating the inelastic spectra centered near (100) in Fe_{1+y}Te , a signature peak for the BOW formation in the monoclinic phase, we observed an acoustic phonon dispersion in both tetragonal and monoclinic phases. While a structural Bragg peak accompanies the mode in the monoclinic phase, in the tetragonal phase Bragg scattering at this \mathbf{Q} is forbidden by symmetry, and we observed no elastic peak. This phonon mode was also observed in superconducting $\text{FeTe}_{0.6}\text{Se}_{0.4}$, where structural and magnetic transitions are suppressed. LDA frozen phonon calculations suggested that this mode could result from a spin imbalance between neighboring Fe atoms, but polarized neutron measurements revealed no additional magnetic scattering. We propose that this “forbidden” phonon mode may originate from dynamically broken symmetry, perhaps related to the strong dynamic spin correlations in these materials.

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