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Ultrafast Structure Control through Nonlinear Phononics MICHAEL FECHNER, Max Planck Institute for the Structure and Dynamics of Matter, DOMENIK M. JURASCHEK, NICOLA A. SPALDIN, Materials Theory, ETH Zurich — Utilizing ultrashort THz light pulses to manipulate the state of matter becomes an emerging approach in condensed matter science. Here we present an approach[1] to actively control the transient structural distortion arising from non-linear phononics in ErFeO3. Using density functional theory, we calculate the structural properties as input to an anharmonic phonon model that describes the response of the system to a pulsed optical excitation. We find that a trilinear coupling of two orthogonal infrared-active phonons to a Raman-active phonon causes a transient distortion of the lattice. The direction of the distortion is determined by the polarization of the exciting light, suggesting a route to nonlinear phononic lattice control and switching. Since the occurrence of the coupling is determined by the symmetry of the system we propose that it is a universal feature of orthorhombic and tetragonal perovskites. Finally, we discuss our findings with respect to experiments of T. Nova et al.[2] as pathway to manipulate the spin system by non-linear phonon excitations. [1] D. M. Juraschek, M. Fechner, and N. A. Spaldin, arXiv 1607.01653 (2016). [2] T. F. Nova, et al., Nature Phys. doi:10.1038/nphys3925 (2016)

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