Theory of non-linear phononics for coherent light-control of solids

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The use of light to control the structural and electronic properties of solids is an area of great current interest. I will present a microscopic theory [1] for ultrafast control of solids with high-intensity Tera-Hertz frequency optical pulses. When resonant with selected infrared-active vibrations, these pulses transiently modify the crystal structure and lead to new collective electronic properties. The theory predicts the dynamical path taken by the crystal lattice using first-principles calculations of the energy surface and classical equations of motion, as well as symmetry considerations.
Two classes of dynamics are identified. In the perturbative regime, displacements along the normal mode coordinate of symmetry-preserving Raman active modes can be achieved by cubic anharmonicities. This validates the mechanism proposed by Först *et al.* [2] and explains the light-induced insulator-to-metal transition of manganites reported experimentally by Rini *et al.* [3]. We also predict a non-perturbative regime in which ultra-fast instabilities that break crystal symmetry can be induced.
Time permitting, I will also describe applications of this theory to the transient crystal structure of $YBa_2Cu_3O_{6.5}$ as measured in time-resolved X-ray diffraction [4].

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