Can you hear the shape of the interatomic potential energy surface?
High-field THz spectroscopy of crystalline systems

Abstract

The interatomic potential energy surface (PES) represents the forces that govern a host of material properties from thermal expansion to phase transitions to energy transport, and yet historically only first-principles computations have been able to access the microscopic details of the PES in solids. Terahertz (THz) electric field pulses with high peak field strengths and relatively low photon energies have proven useful in observing fascinating effects in a number of materials, including exciting vibrations to large amplitudes to sample anharmonic regions of the PES [1]. Further potential examples of THz control over material properties have been suggested and even modeled, such as ultrafast polarization switching by soft mode excitation [2]. Dynamic control over a crystal lattice using high-field THz pulses in order to influence material properties, study the potential energy surface, and track coherent energy flow in a system is a promising and still relatively unexplored area of study.

By utilizing intense pulses of terahertz radiation, we excite phonon modes in solids to extreme amplitudes, allowing us to investigate anharmonic regions of the PES. Early results from my group have shown that experimental determination of the PES is possible [1], and new results are revealing the intricacies of nonlinear excitation by probing multiple vibrational degrees of freedom simultaneously.

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