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Theory of pump-probe spectroscopy: Ultrafast laser engineering of ordered phases and microscopic couplings

Intense femtosecond laser pulses, spanning a large range of photon energies from the X-ray to the THz regime, allow for controlled excitations ("pump") and monitoring ("probe") of the nonequilibrium dynamics of all the relevant microscopic degrees of freedom in solids. The field of ultrafast materials science is currently evolving from measuring time constants - for instance for the decay of hot electrons via phonon emission - towards ultrafast laser engineering of nonthermal phases of matter with novel properties. Notable examples include light-induced superconducting-like behavior [1], ultrafast switching to hidden ordered states [2], or time-reversal symmetry-broken Floquet states in topological insulators [3].

I will discuss recent theoretical progress in understanding these diverse phenomena from microscopic models and nonequilibrium simulations. I will show examples of light-enhanced superconductivity in an electron-phonon system from classical nonlinear phononics [4,5] and laser-controlled order competition between superconductivity and charge-density waves [6]. I will discuss laser engineering of microscopic couplings in graphene [7] based on quantum nonlinear phononics [8,9]. I will also show ab initio time-dependent density functional theory results for laser-engineered Hubbard U in NiO [10], with a recent application to light-induce the elusive magnetic Weyl semimetal in pyrochlore iridates [11].

I will also highlight some recent developments towards cavity quantum electrodynamical environments enhancing electron-phonon coupling in 2D materials [12], and efforts to make nonequilbrium Green's functions fast for correlated ordered phases (excitonic condensates) using the generalized Kadanoff-Baym ansatz [13].

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