The limits of electronic, optical and thermal performance of these materials are determined by their atomic-scale dynamics. In order to surpass conventional, bulk properties of materials, an accurate description of excited-state phenomena is essential. Light-matter interactions and electronic excited-state phenomena require high-level electronic structure methods beyond the all-pervasive density-functional theory. Simultaneously, the properties of interest are fundamentally non-equilibrium and require techniques that are reliable beyond small perturbations from equilibrium. Electron-photon, electron-electron as well as electron-phonon dynamics and far-from-equilibrium transport are critical to describe ultrafast and excited-state optoelectronic interactions in materials. \textit{Ab initio} descriptions of phonons are essential to capture both excitation and loss (decoherence) mechanisms, and are challenging to incorporate directly in calculations due to a large mismatch in energy scales between electrons and phonons. In this talk I will show the first results using a new theory method we have developed to calculate arbitrary electron-phonon and electron-optical interactions in a Feynman diagram many-body framework integrated with a nonequilibrium carrier transport method (NESSE). Further, I will discuss a new formalism at the intersection of cavity quantum-electrodynamics and electronic structure methods, quantum-electrodynamical density functional theory (QEDFT), to treat electrons and photons on the same quantized footing. Finally, I will demonstrate how phonons are formally included in QEDFT to predict new single molecule - cavity optomechanical effects.