Abstract Submitted
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Coupled dynamics of electron quasiparticles, the electromagnetic field, and nuclear motion in complex systems[1] ROLAND ALLEN, Texas A&M University, XIANG ZHOU, Texas A&M University, Wuhan University, MENG GAO, Texas A&M University, CHENWEI JIANG, Texas A&M University, Xi'an Jiaotong University, ZHIBIN LIN, Texas A&M University, Colorado School of Mines, REMRSEC — A vast number of problems in physics, chemistry, biology, and engineering involve the coupled dynamics of electrons and ions in materials and molecules, and their interaction with the radiation field. Here we review some recent work by the present investigators in both developing new techniques to address these problems and performing detailed simulations for systems that are currently of intense interest – for example, graphene and carbon nanotubes. The new theoretical ideas focus largely on (1) the inclusion of many-body effects (through e.g. a time-dependent GW self-energy) and (2) the use of the Kadanoff-Baym equations for nonequilibrium Green's functions. We will derive a time-dependent quasiparticle equation, which is the time-domain and nonequilibrium version of the well-known frequency-domain and equilibrium quasiparticle equation derived by Hedin and subsequently used by many groups (to obtain e.g. the correct band gaps of semiconductors).

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