Towards ab initio simulations of driven and non-equilibrium systems through novel theoretical and numerical approaches

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In this talk, I will discuss the recent developments in the many-body perturbation theory in Green's function formulation, aiming to capture the (driven) dynamical correlations in realistic nanoscale condensed matter systems. Compared to the equilibrium methods, the out-of-equilibrium phenomena suffer from additional computational and theoretical bottlenecks manifested through the time non-local terms, leading to prohibitively costly simulations using the common condensed matter electronic structure approaches. I will, in particular, focus on overcoming these hurdles in non-equilibrium dynamics calculations and the possible truncations and reformulations of time-nonlocal quantum interactions. I will present numerical and data-driven methods, as well as a novel real-time Dyson expansion formalism that captures the non-equilibrium physics of driven systems exhibiting emergent quasiparticle phenomena. Among other advantages, it can be readily deployed together with real-time random sampling approaches, which revolutionized the calculations employing Green's function formalism and allow simulations of systems with tens of thousands of electrons at GW and post-GW levels.