

Nonequilibrium electrons coupled with phonons and collective orders

The study of nonequilibrium phenomena in correlated materials has recently become one of the most active and exciting branches of condensed matter physics. This is largely due to advances in light sources and time-resolved spectroscopies on the ultra-short time scales, which made it possible not only to observe and describe but also to design systems with new remarkable properties by coupling them to external electromagnetic fields.

The goal of this project is to study correlation between electrons, phonons, excitons and other quasiparticles in excited quantum states of matter. The behavior of atomic, molecular and solid state systems interacting with laser fields on the femtosecond time-scale will be investigated with the help of nonequilibrium Green's function approach also known as quantum kinetics. In novel quantum materials, the vastly different energy and time scales and the quantum nature of the involved bosonic particles pose considerable challenges for theory. Therefore, we will exploit our recently developed (2021) time-linear formalism for solving quantum kinetics equations using the so-called generalized Kadanoff-Baym ansatz. Some striking applications to photoinduced dynamics of organic molecules, carrier and exciton dynamics in 2D materials and electron-phonon thermalization have already been demonstrated. However, we are just at the beginning of these exciting developments of making the method a practical and versatile tool for multiscale real-world applications. My objective is to extend the method towards new materials such as excitonic insulators, strongly-correlated and magnetically-ordered systems and to expand the spatial and time ranges of time-resolved first principles simulations.

This will improve our understanding of excited quantum states of matter. In a long time perspective they may lead to practical applications having a huge societal impact. Numerous applications in photovoltaics, superconductivity, and molecular electronics are expected.