Probing non-equilibrium dynamics in correlated materials with first-principles-based time-dependent microscopic models

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The interaction between charge, spin, and lattice degrees of freedom in strongly correlated systems under external stimuli leads to several intriguing phenomena. High-resolution ultrafast pump-probe spectroscopy experiments in these materials have uncovered fascinating physical effects, such as photoinduced phase transitions, photovoltaic effects, and transient "hidden" phases. However, the fundamental mechanisms behind these photoinduced processes, which are vital for practical applications, remain largely unknown. A detailed microscopic understanding of the energy conversion processes is crucial. Theoretical investigation of these processes is complex and requires methods capable of addressing the large spatiotemporal scales of various active degrees of freedom. I will discuss the first-principles-based microscopic modeling of relaxation dynamics in materials and present simulation results for correlated oxides, emphasizing the role of spin and phonons in photo-induced dynamics. In the charge-ordered stripe phase, photoinduced phase transitions can be highly selective based on the light pulse's intensity and polarization. I will present simulation results on the generation and evolution of photocurrent, along with strategies to enhance the photovoltaic response in strongly interacting ferroelectric systems. I will also briefly highlight possible spin- and lattice-assisted relaxation mechanisms.

References:

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