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Theoretical Modeling of Ultrafast Phase Transitions from the Femtosecond to the Picosecond Scale

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In this talk, I will introduce a theoretical approach to ultrafast phase transitions able to capture both the electron and phonon dynamics after laser pumping on a time scale ranging from a few femtoseconds to several picoseconds after laser irradiation.

At short times, the method relies on the solution of the Bloch equations coupled to the Ehrenfest dynamics. It includes the electric field of the pump as well as the electron-phonon, electron-electron, and phonon-phonon scattering completely from first principles.

At longer times before recombination, when the electron-electron interaction generates a photoexcited quasi-equilibrium electron-hole plasma, the approach is based on a constrained density functional perturbation theory (cDFPT) scheme accounting both for the presence of holes in the valence band and electrons in the conduction band (two Fermi levels approach). In this framework, calculation of forces, phonon dispersion, and electron-phonon coupling are possible, as well as molecular dynamics with machine learning potential in the presence of an electron-hole plasma.

I will showcase the application of the method to several materials ranging from low-dimensional dichalcogenides to ferroelectrics and thermoelectrics.

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