Abstract:
Recent developments showed that femtosecond (0.000 000 000 000 001 s)-laser pulses are an ideal tool to address and/or manipulate properties in matter, since pulse durations are comparable to typical time scales of atomic motions in molecules and solids. The optical energy of such an excitation is deposited mainly in the electronic system, because of the high difference in the coupling strength of light to electrons and atoms. Therefore, electronic temperatures of several $10^5$ K can be induced, whereas the atomic system remains almost unaffected near its initial temperature. This extreme nonequilibrium conditions have a direct influence on the bonding properties of the material and are the driving force to a variety of laser-induced ultrafast phenomena like coherent phonons, thermal phonon squeezing, solid-to-solid phase transitions, and solid-to-liquid phase transitions. In order to resolve the atomic pathways and the energy flow during these structural responses, we performed ab initio molecular dynamics simulations for materials in bulk, thin film and 2D geometries. In this talk we will introduce some of the above mentioned phenomena and have a closer look at physical mechanisms on a femtosecond-time scale. Moreover, the knowledge of these physical mechanisms will allow us to propose a structural control mechanism in the high excitation regime.