Molecular Nano(Newton)Mechanics

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The manipulation of covalent bonds in molecular systems using mechanical forces became possible only during the last decade. Several experimental advances made possible the site-specific application of forces in the nano-Newton range required to break or make chemical bonds. Much in parallel with experimental advances, theoretical approaches were developed which pave the way to understanding these phenomena.

My lecture will give an overview of our efforts to unveiling the nanomechanical properties of hybrid molecule/metal junctions and of force-induced reactions, including optomechanical switching, in the condensed phase.

Can we predict HIOS crystal structures by classical molecular computer simulations?

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A necessary prerequisite for the modeling and rationalization of HIOS's functional properties is the knowledge of the molecular arrangement of the conjugated organic molecules (COMs), that is, their inhomogeneous, mesoscale crystal structure at the hybrid interface. In this talk I first try to briefly review some of the challenges in the theoretical prediction of (liquid) crystalline structures of COMs in bulk and then introduce potential routes of prediction by using classical molecular computer simulations. A case study on the well-characterized para-sexiphenyl (6P) bulk crystals will be discussed in more detail. Finally an outlook on the application and

extension of the simulation methods to other COMs and HIOS is provided.