Dynamical Simulations of Materials Under Extreme Conditions
Across Multiple Time and Length Scales

Atomistic simulations are a crucial tool for investigating the behavior of materials under extreme conditions, including mechanical extremes like shock, high pressure and temperature regimes, or irradiation. Experiments are typically difficult to perform under such conditions, and often unable to provide detailed insight into fundamental processes important for developing physics-based models of these systems. As one example, simulations allow us to identify the chemical reactions leading to the detonation of an energetic material, and provide the missing link between reactants and products. With advances in algorithms and methods that push the time and length scales accessible via direct atomistic simulation, the choice of the simulation technique is guided by three main criteria: the time scale one is interested in, the size of the system to be studied, and the accuracy required to provide quantitative results. I will highlight fundamental methods development as well as applications to a spectrum of materials. These include the development of the SED-REBO potential for the simulation of highly strained carbon materials, combined DFT and empirical studies of point defects and fission products diffusion in UO2, and the application of accelerated molecular dynamics to the study of mass transport in disordered complex oxides. Finally, I will describe recent work on validating DFTB models for energetic materials and their application to quantifying T- and P-dependent reaction rates in thermodynamic conditions pertinent to detonation.