Atomistic simulations for Energized Processes in the Gas Phase

Markus Meuwly,[1] *University of Basel*

In this contribution I will discuss the use of classical and quantum simulations to characterize small molecular systems based on accurate potential energy surfaces. Starting from high-quality ab initio calculations the data is represented either as a parametrized force field or a reproducing kernel Hilbert space for efficient calculation of energies and forces. Using this as input to classical or quantum simulations, relevant spectroscopic or dynamical observables are determined to validate the simulations and predict properties inaccessible to direct experimentation. They include, for example, equilibrium rates of bimolecular reactions or vibrational relaxation times at very high temperatures.

[1] m.meuwly@unibas.ch