Machine Learning for Reactive Molecular Dynamics

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Following chemical reactions at atomic resolution is one of the formidable challenges in physical chemistry. Ab initio MD simulations are an attractive possibility to do this and Prof. Hase has been at the forefront of this effort. Alternatively, empirical or – more recently - machine-learned models for the potential energy surfaces have been developed and used. Realistic computer modeling of chemical reactions requires means to follow bond-breaking and bond-formation processes based on high-quality representations of the reaction energetics. I will discuss our approach to address this problem using either multi-state reactive MD or machine-learned energy functions based on neural networks or reproducing kernel representations. Examples ranging from three-atom reactions at high temperatures to ligand binding reactions in proteins will be presented and the insights into atomistic details of the reactions will be discussed.