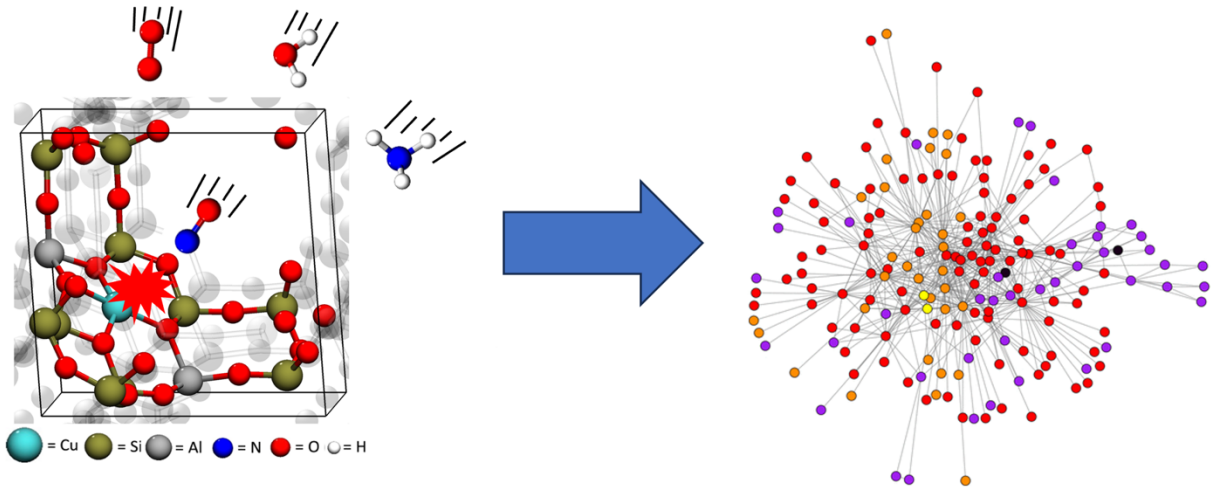
Computational Reaction Discovery and Construction of Reaction Networks

Jan Meisner

Institute for Physical Chemistry, Heinrich Heine University Düsseldorf, Düsseldorf



Recent developments of efficient computational methods make it possible to discover chemical reactions starting from basic principles and elucidate novel reaction mechanisms that might otherwise have been overlooked. Entire reaction networks can be discovered autonomously, which enables a complete investigation of chemical systems with all their elementary steps, intermediates, and side reactions. In this talk, modern approaches for the computational discovery of chemical reactions are presented. The capabilities of *ab initio* molecular dynamics accelerated by different external forces, coined nanoreactor molecular dynamics (NMD), [1] are demonstrated and improvements of reaction network construction and visualization are shown. [2,3] Recent studies span the fields of combustion chemistry, atmospheric chemistry, and catalysis. [3,4]

The extension of NMD to periodic systems also allows the investigation of surface reactions and porous media. Here, an application of periodic NMD simulations to construct a complex reaction network for zeolite catalysis in the context of Selective Catalytic Reduction (SCR) is given, which elucidates the reaction mechanism of the unwanted SCR side reaction of N_2O formation.

[1] L.-P. Wang *et al.*, *Nat. Chem.*, **2014**, 6, 1044-1048
[2] J. A. Meissner, J. Meisner, *J. Chem. Theory Comput.*, **2025**, 1, 218-229
[3] P. Kuboth *et al., J. Chem. Inf. Model.,* 2025, accepted, DOI: 10.1021/acs.jcim.4c02106
[4] R. Xu *et al., Chem. Sci.*, **2023**, 14 (27), 7447-7464
[5] D. Deißenbeck *et al., in preparation*