C10

Reaction Discovery in Periodic Systems

J. Meisner[1], D. Deißenbeck[1], S. Ralf[1], W. A. Kopp, [1], P. Meier[1]

[1] *Heinrich Heine University Düsseldorf, Germany*

Recent developments of efficient computational methods make it possible to discover chemical reaction networks starting from basic principles and elucidate novel reaction mechanisms that might otherwise have been overlooked. In this talk, the improvements of ab initio nanoreactor molecular dynamics (NMD) [1] are demonstrated. [2,3] The extension of NMD to periodic systems also allows the investigation of surface reactions and porous media. Among others, an application of periodic NMD simulations to construct a complex reaction network for zeolite catalysis is given, which elucidates the reaction mechanism of the unwanted side reactions in the Selective Catalytic Reduction of N2O formation.[4]

[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 65, 7, 3127–3136.
[4]D. Deißenbeck et al., Angewandte Chemie 2026, 65(6), p.e14074.