

## Operando Computational Catalysis

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A key focus in heterogeneous catalysis is to understand the dominant reaction paths and isolate the character of the active site. This is challenging because of the dynamic character of the catalyst, which may undergo structural and phase changes as a response to the reaction conditions. This stresses the importance to perform physical and chemical characterization of catalysts during operando conditions. This applies also to computational work, aiming at establishing links between elementary steps and catalyst activity.

In this presentation, I will discuss our recent efforts to understand CO and methane oxidation over palladium and platinum using first principles calculations exemplifying different aspects of kinetic simulations based on theoretical data [1-4]. Special attention will be given the attempt to perform explicit simulations of reaction kinetics over metal nanoparticles. These simulations reveal that kinetic couplings between different sites on the particles largely determine the overall catalytic activity. Our results show that it is rather the site-assembly than a special site that determines the activity.

- [1] M. Jørgensen, H. Grönbeck, ACS Catalysis 6, 6730 (2016).
- [2] M. Van den Bossche and H. Grönbeck, J. Am. Chem. Soc. 137, 12035 (2015).
- [3] M. Jørgensen, H. Grönbeck, ACS Catalysis 7, 5054 (2017).
- [4] M. Jørgensen, H. Grönbeck, Angew. Chem. Int Ed. **57**, 5086 (2018).