O 48: Overview Talk: Henrik Grönbeck

Time: Wednesday 9:30–10:15 Location: H15

Invited Talk O 48.1 Wed 9:30 H15

Catalytic activity from first principles - towards operando computational catalysis — •Henrik Grönbeck — Chalmers University of Technology, Göteborg, Sweden

A key focus in heterogeneous catalysis is to understand the dominant reaction paths and isolate the character of the active sites. This is a challenge because of the dynamic character of the catalyst, which may undergo structural and phase changes as a response to the reaction conditions. To obtain information on the active site, the catalyst should preferably be characterized during operando conditions. The need to account for reaction conditions holds also computational work with the purpose to establish 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 [1-5] exemplifying different aspects of operando computational catalysis. Special attention will be given our attempt to perform explicit simulations of reaction kinetics over metal nanoparticles. The examples will cover how composition, size, shape and strain may affect the catalytic turn over frequency.

[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). [5] T. Nilsson Pingel, M. Jørgensen, A. Yankovich, H. Grönbeck, and E. Olsson, Nature Comm. 9, 2722 (2018).