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Probing the Surfaces of Nanostructures under Reactive Environments

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Nanostructures represent an interesting class of materials. Especially their surfaces which to a large extent govern the functionality of these materials are of fundamental interest. For example, the activity of heterogeneous catalysts strongly rely on the structure of these surfaces. The nature of these surfaces is a strong function of the conditions to which the nanoparticle is exposed, i.e. surrounding gases and the temperature. Detailed quantitative information of the surfaces under operating conditions is inherently difficult to access due to limitations of characterization equipment. Advances in electron microscopy such as MEMS heaters and reaction cells and fast cameras have provided new possibilities for *in situ* characterization at the atomic scale (1). Applied in combination with newly developed automated analysis techniques, strong and robust characterization of nanoparticle dynamics can be achieved. However, automated image analysis does have its pitfalls. Knowledge of imaging conditions is a necessary prerequisite in order to extract meaningful results.

Here we show examples from recent studies of catalytically relevant materials using these new possibilities. Among these, gold and platinum nanoparticles and iron oxides. We investigated the surface structure and dynamics of gold nanoparticles under varying atmospheres. Using environmental high-resolution transmission electron microscopy, gold nanoparticles supported on cerium dioxide have been imaged under varying conditions. The data is analyzed using automated real-space peak finding algorithms and convolutional neural networks developed in-house.

Figure 1 shows some of the observations in varying environments. These observations indicate that as expected, different gas molecules interact differently with different facets.

These observations highlight the advantages of automated analysis and strongly suggest that the catalytically active surfaces are dynamic rather than static entities.

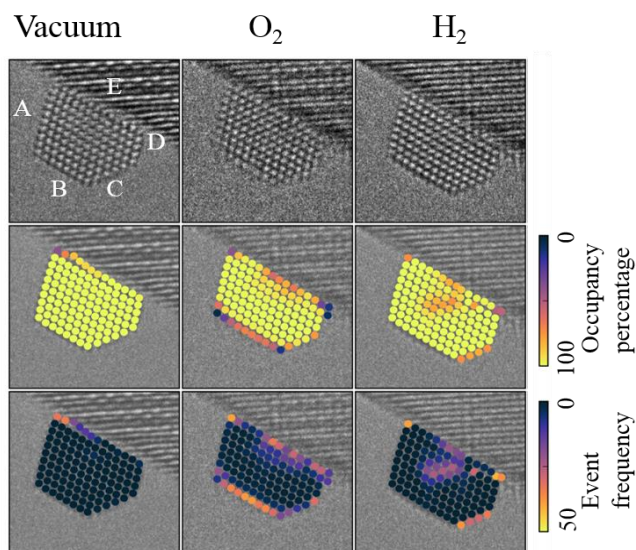


Figure 1: Quantification of occupancy and hopping frequency on the surface of a gold nanoparticle at room temperature.

1. T. W. Hansen, J. B. Wagner, Eds., *Controlled Atmosphere Transmission Electron Microscopy*, (Springer, 2016), pp. 329.
2. J. Madsen, P. Liu, J. B. Wagner, T. W. Hansen, J. Schiøtz, Accuracy of surface strain measurements from transmission electron microscopy images of nanoparticles. *Adv. Struct. Chem. Imag.* 3, 12 (2017).