

Séminaire **SOLEIL**

Reversible shape changes of oxide supported metal nanoparticles under oxidizing and reducing conditions

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Invité par Alina VLAD

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Grand Amphi SOLEIL**

Chemical reactions on supported metal nanoparticles are important for a wide range of applications, such as heterogeneous catalysis, exhaust gas cleaning or energy conversion. In the last decades, basic surface science studies have helped to understand the interaction of gases with single crystal metal surfaces at near ultra-high vacuum pressures. These results are however not directly applicable to metal nanoparticles since these exhibit additional degrees of freedom, such as under-coordinated atoms at corners and edges, reduced, nano-sized dimensions of differently oriented, communicating facets and an interface with the support.

To gain atomistic insight into the shape, size and structure of nanoparticles under reaction conditions, we developed a novel formalism based on the quantitative analysis of x-ray reciprocal space maps from epitaxial nanoparticles on single crystal oxide supports. As a result, we obtain the average particle shape and size, which can be studied in-situ at near-atmospheric pressures and elevated temperatures. During my presentation, I will compare the oxidation and reduction behavior of MgO(100) supported Rh and Pd nanoparticles from 10^{-5} mbar to 10 mbar gas pressures. For Rh nanoparticles, low index facets are stabilized by the formation of ultrathin surface oxides, which can be directly identified from their diffraction fingerprint [1]. In contrast, Pd particles exhibit a shape transformation to higher index facets under oxygen exposure [2]. For both systems particle shapes will be compared to predictions by a density functional theory based Wulff construction as a function of the surrounding gas atmosphere [3].

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References:

- [1] P. Nolte, A. Stierle, N. Y. Jin-Phillipp, N. Kasper, T. U. Schulli, H. Dosch, *Science* 321, 1654 (2008).
- [2] P. Nolte, A. Stierle, N. Kasper, N. Y. Jin-Phillipp, N. Jeutter, H. Dosch, *Nanoletters* (2011) dx.doi.org/10.1021/nl2023564
- [3] F. Mittendorfer, N. Seriani, O. Dubay, G. Kresse, *Phys. Rev. B* 76, 233413 (2007).



Ce séminaire sera suivi d'une pause-café

Formalités d'entrée : accès libre dans l'amphi du Pavillon d'Accueil. Si la manifestation a lieu dans le Grand Amphi Soleil du Bâtiment Central, merci de vous munir d'une pièce d'identité (à échanger à l'accueil contre un badge d'accès).