

# Reactions at oxide surfaces and oxide/metal interfaces

Henrik Grönbeck<sup>1</sup>

<sup>1</sup>*Department of Physics and Competence Centre for Catalysis, Chalmers University of Technology,  
SE 41296 Göteborg, Sweden  
ghj@chalmers.se*

Metal oxides is a wide class of materials that are used in numerous applications where heterogeneous catalysis is but one example. Oxides are in catalysis employed as supports for the active phase, storage materials and catalysts. Given the wide range of applications, it is important to explore general phenomena of oxide chemistry. In this contribution, we will discuss different aspects of reactions on oxide surfaces and oxide/metal interfaces. The results are based on density functional theory calculations and first principles microkinetic modelling.

Open-shell molecules frequently display cooperative adsorption mechanisms on oxides, where pairs of adsorbates are significantly more stable than the isolated species. We discuss this for a range of oxides and adsorbate pairs [1]. The pairing energy is found to be a convoluted measure of charge transfer energies, electrostatic interactions, and ionic relaxations. Adsorbate pairing has marked effects on the reactivity, which is exemplified by a detailed analysis of methane oxidation over palladium oxide [2]. A related charge transfer phenomenon is the possibility to tune adsorption properties for ultrathin oxide films supported on metals [3]. We will also discuss the case without charge transfer where the properties of thin oxide films still can be tuned by the choice of support metal [4].

Oxide phases can be formed *in situ* from metal alloys during oxidation reactions. This will be discussed in connection to CO oxidation over Pt<sub>3</sub>Sn where the formation of an SnO<sub>2</sub> phase supported on Pt and the reaction taking place at the SnO<sub>2</sub>/Pt interphase may explain the low temperature activity of this system [5].

## References:

- [1] M. Van den Bossche, H. Grönbeck, *J. Phys. Chem. C* **120**, 8390 (2017).
- [2] M. Van den Bossche, H. Grönbeck, *J. Am. Chem. Soc.* **137**, 12035 (2015).
- [3] A. Hellman, S. Klacar, H. Grönbeck, *J. Am. Chem. Soc.* **131**, 16636 (2009).
- [4] L.R. Merte, C.J. Heard *et al.* *Angew. Chem. Int. Ed.* **55**, 9267 (2016).
- [5] M. Vandichel, A. Moscu, H. Grönbeck, *ACS Catalysis* **7**, 7431 (2017).