

## PREDICTING THE REACTIVITY OF TRANSITION METAL SURFACES SIMPLY BY COUNTING ATOM NEIGHBORS

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Heterogeneous catalysis is at the core of sustainable chemistry, since it allows a fine control of chemical bond forming and breaking processes. For the optimal design of catalysts, a fundamental atomic scale understanding of the structure and electronic structure of the catalytic particle, in interaction with the reactant is of utmost importance. Computational chemistry today is a key method, to reach such an understanding at the molecular level of the structure of the active site and of the elementary processes occurring during the catalytic act.

The understanding of the catalytic properties of nanoparticle catalysts and the design of optimal composition and structures demands fast methods for the calculation of adsorption energies. By exploring the adsorption of O and OR (R=OH, OOH, OCH<sub>3</sub>) adsorbates on a large range of surface sites with 9 transition metals, we propose new structure sensitive scaling relations between the adsorption energy of two adsorbates that are valid for all metals and for all surface sites.<sup>1</sup> This opens the way for a new class of activity volcano plots where the descriptor is not an energy but a structure-related descriptor. In addition, to better grasp finite size effects in the nanoparticles, a generalized coordination number is proposed as a leading descriptor for the adsorption strength.<sup>2,3</sup> In the case of oxygen reduction reaction, we show that only surfaces and nanostructures with generalized coordination larger than that of the Pt(111) surface, and hence concave defects, can surpass the activity of Pt(111), whereas convex defects are inactive.<sup>3,4</sup>

Simple structural descriptors as generalized coordination show hence a strong predictive potential for the in-silico design of optimal catalysts.

### References

1. F. Calle-Vallejo, D. Loffreda, M. T. M. Koper and P. Sautet, *Nature Chemistry*, 2015, **7**, 403-410
2. F. Calle-Vallejo, J. I. Martínez, J. M. García-Lastra, P. Sautet and D. Loffreda, *Angewandte Chemie International Edition* 2014, **53**, 8316-8319
3. F. Calle-Vallejo, J. Tymoczko, V. Colic, Q. H. Vu, M. D. Pohl, K. Morgenstern, D. Loffreda, P. Sautet, W. Schuhmann, A. S. Bandarenka, *Science*, 2015, **350**, 185-189
4. F. Calle-Vallejo, M. D. Pohl, D. Reinisch, D. Loffreda, P. Sautet, A. S. Bandarenka, *Chem. Sci.*, 2017, **8**, 2283-2289