Seminar

Konstantin Neyman

ICREA and Universitat de Barcelona, Barcelona, Spain

Wednesday, 20th March 2024, 16:00 s.t.
TU Wien, Institut für Materialchemie, E165, 1060 Wien, Lehargasse 4
Building BC, 1st Floor, Seminar Room Lehar 1

Computational Modelling of Bimetallic Nanoparticles

Bimetallic nanoparticles (nanoalloys) are common materials of choice for various applications. However, determining the chemical ordering in nanoalloys, which often defines their properties, is very challenging. We developed a method to determine the lowest-energy chemical (atomic) orderings in nanoalloys by first-principles Density Functional Theory (DFT) calculations combined with a Topological (TOP) approach [1,2]. The method allows one to efficiently predict the most stable ordering patterns of atoms in bimetallic crystallites comprising up to thousands atoms. So far the applications of the method have been focused on nanoalloys used in catalysis and energy technologies, for which surface atomic ordering is key for the reactivity. Among the studied nanoalloys were PtCo [3,4], PtNi [5], CuNi [6], PdRh [7], PdX [1,2], PtX (X = Au, Ag, Cu) [8,9].

Our method to calculate chemical orderings will be outlined and its applications illustrated by results for catalytically relevant bimetallic nanoparticles. This modelling method helps to accelerate design of tailor-made bimetallic nanoalloys for various technological needs. It also allows deepening general understanding of the chemical bonding in nanoalloys and their reactivity.

References

1. S.M. Kozlov et al. How to determine accurate chemical ordering in several nanometer large bimetallic crystallites from electronic structure calculations. *Chem. Sci.* 6 (2015) 3868
2. G. Kovács et al. Versatile optimization of chemical ordering in bimetallic nanoparticles. *J. Phys. Chem. C* 121 (2017) 10803
3. G. Kovács et al. Revealing chemical ordering in Pt-Co nanoparticles using electronic structure calculations and X-ray photoelectron spectroscopy. *Phys. Chem. Chem. Phys.* 17 (2015) 28298
4. M. Vorokhta et al. Surface composition of magnetron sputtered Pt-Co thin film catalyst for proton exchange membrane fuel cells. *Appl. Surf. Sci*. 365 (2016) 245
5. I. Khalakhan et al. Irreversible structural dynamics on the surface of bimetallic PtNi alloy catalyst under alternating oxidizing and reducing environments. *Appl. Catal. B: Environ.* 264 (2020) 118476
6. A. Wolfbeisser et al. Surface composition changes of CuNi-ZrO2 catalysts during methane decomposition: An operando NAP-XPS and density functional study. *Catal. Today* 283 (2017) 134
7. L. Vega et al. Using density functional calculations to elucidate atomic ordering of Pd-Rh nanoparticles at sizes relevant for catalytic applications. *Chin. J. Catal.* 40 (2019) 1749
8. L. Vega et al. Chemical ordering in Pt-Au, Pt-Ag and Pt-Cu nanoparticles from density functional calculations using a topological approach. *Mater. Adv*. 2 (2021) 65
9. X. Xie et al. Optimal Pt-Au alloying for efficient and stable oxygen reduction reaction catalyst. *ACS Appl. Mater. Interfaces* 15 (2023) 1192

All interested colleagues are welcome to this seminar lecture
(45 min. presentation followed by discussion).

Günther Rupprechter
Director of Research

André Vogel
Coordinator