

Oxide formation and structure at platinum-tin alloy surfaces

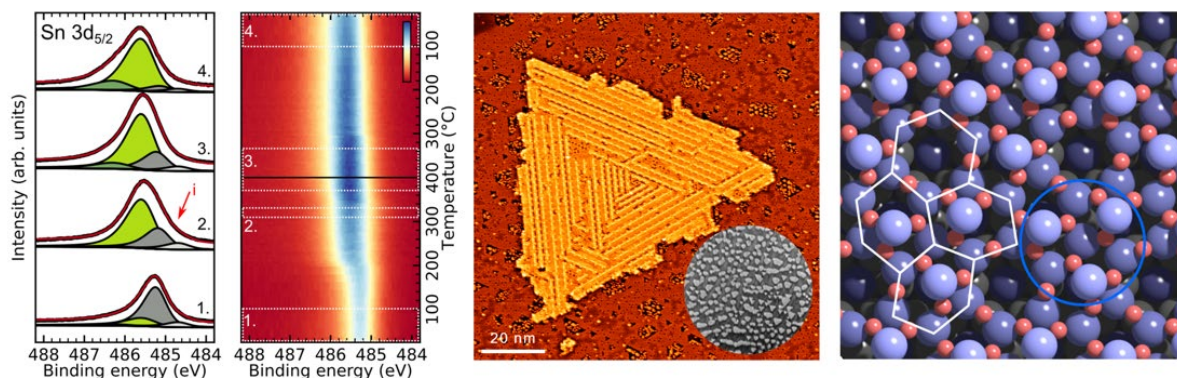
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Oxides of variable valence are common promoters for platinum-group catalysts, often lowering the onset temperatures for oxidation reactions, reducing poisoning effects and improving selectivity. The increased complexity brought about by addition of such an oxide is substantial, however, and makes detailed structure-reactivity relationships very challenging to obtain. Tin-promotion of platinum catalysts is a good case in point; though known for years as an active material for e.g. PROX and alcohol electrooxidation, the reasons for this are still unclear. The challenges involved are also commonly encountered: the chemical state of tin evolves dynamically during reactions, depending on temperature and the gas composition, making the 'active state' difficult to pinpoint and to study in detail and the structures of ultra-thin oxides of tin are varied and complex, even on the simplest low-index surfaces, and until recently were completely unsolved.

Progress in overcoming these challenges requires a broad approach including in situ methods for characterization of the materials under realistic conditions as well as high-precision surface structure analysis under UHV, supported by ab initio theoretical modelling. We present here an overview of our efforts in this direction, including studies using ambient-pressure XPS [1,2] and grazing-incidence XAFS [3] measured during CO oxidation, and surface X-ray diffraction and high-precision low-energy and scanning probe microscopy measured under UHV conditions [4,5,6]. Despite a wealth of experimental information about the surface oxide phases formed on these surfaces, their atomic structures could still not be determined directly. DFT-based structure search, aided by machine learning, was able to produce candidate structures that could be verified by experiment, however [4]. The use of these global search methods, alongside state-of-the art characterization, is argued to be essential to further progress in this area.



- [1] H.J. Wallander et al., J. Phys. Chem. C, **126**, 6258–6266. (2022)
- [2] H.J. Wallander et al., Submitted.
- [3] H.J. Wallander et al., In Preparation.
- [4] L.R. Merte et al., Angew. Chem. Int. Ed. **61**, e202204244. (2022)
- [5] L.R. Merte et al., J. Phys. Chem. C **127**, 2988–2994. (2023)
- [6] N. Braud et al., In Preparation.