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Seminar

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TU Wien, Institut für Materialchemie, E165, 1060 Wien, Lehargasse 4
Building BC, 1st Floor, Seminar Room Lehar 1

Unraveling the Secrets of Nanoporous Gold: A Theoretical Investigation of its Surface Properties and Catalytic Behavior

Nanoporous gold (np-Au) has recently emerged as a highly selective catalyst, potentially suitable for green and low-temperature applications.[1] In contrast to the more extensively studied gold nanoparticle catalysts, the mechanistic understanding of catalytic processes on pristine and oxide-coated np-Au is far less developed. In this work the activation of O_2 and the formation of quasi-ordered oxygen chain structures on nanoporous gold have been studied by DFT calculations, microkinetic modeling, and *ab initio* molecular dynamics (AIMD) simulations.[2-4]

Modern surface science has revealed that a catalyst is not a rigid body, but undergoes rapid (sometimes irreversible) dynamic changes during chemical processes occurring on its surface. Many theoretical studies still use an oversimplified model of a metal catalyst as a rigid, clean, and perfect surface. In addition to applying traditional "static" DFT calculations, this work theoretically investigates the dynamic processes occurring on the surface of np-Au in response to changes in the chemical environment using *ab initio* molecular dynamics (AIMD) simulations. We will present new insights into the mechanisms of oxidation catalysis, in particular the O_2 activation step, on pristine and ceria-coated np-Au as revealed by first-principles based modeling studies.

References

1. Wittstock, G.; Bäumer, M.; Dononelli, W.; Klüner, T.; Lührs, L.; Mahr, C.; Moskaleva, L. V.; Oezaslan, M.; Risse, T.; Rosenauer, A.; Staubitz, A.; Weissmüller, J.; Wittstock, A. *Chem. Rev.* **2023**, *123*, 6716-6792. DOI: 10.1021/acs.chemrev.2c00751.
2. Dononelli, W.; Tomaschun, G.; Klüner, T.; Moskaleva, L. V. *ACS Catal.* **2019**, *9*, 5204-5216. DOI: 10.1021/acscatal.9b00682.
3. Li, Y.; Li, S.; Bäumer, M.; Ivanova-Shor, E. A.; Moskaleva, L. V. *ACS Catal.* **2020**, *10*, 3164-3174. DOI: 10.1021/acscatal.9b05175.
4. Li, Y.; Li, S.; Bäumer, M.; Moskaleva, L. V. *J. Phys. Chem. C* **2021,** *125*, 26406-26417. DOI: 10.1021/acs.jpcc.1c07040.

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

Günther Rupprechter
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