NITheCS

National Institute for
Theoretical and Computational Sciences

NITheCS COLLOQUIUM:

What Makes Nanoporous Gold a Unique Catalyst? Insights from Modelling Studies of its Surface Chemistry

Prof Lyudmila Moskaleva (University of the Free State)

Monday, 6 November 2023 | 16h00 – 17h00 SAST

Venue: in person* and online

** Neelsie Cinema, Stellenbosch University*

--- Cheese and wine will be served at the venue ---

ABSTRACT

Nanoporous gold (np-Au) has recently emerged as a highly selective catalyst, potentially suited to environmentally friendly 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. This work studied the activation of O_2 on nanoporous gold by DFT calculations, microkinetic modelling, and *ab initio* molecular dynamics (AIMD) simulations.[2-4]

In our computational study on the basis of DFT (PBE-PAW) we used stepped Au(321) and Au(221) surfaces as periodic slab models to represent curved ligaments of np-Au. In addition to traditional "static" DFT computations, microkinetic modelling and AIMD simulations were used as computational tools.

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 models, this work theoretically examines dynamic processes occurring on the surface of np-Au in response to changes of the chemical environment by using ab initio molecular dynamics (AIMD) simulations. We will present new insights into the mechanisms of oxidation catalysis, specifically the O_2 activation step, on pristine and ceria-coated np-Au revealed by first-principles based modelling 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.

BIOGRAPHY

Lyudmila V. Moskaleva is an Associate Professor in the Department of Chemistry at the University of the Free State. She received her PhD in Physical Chemistry in 2001 from Emory University, USA, and her MSc in Chemistry in 1997 from the Higher Chemical College of the Russian Academy of Sciences, Russia. In 2002-2006 she was an Alexander von Humboldt Research Fellow and a postdoctoral fellow at Technische Universität München, Germany. From 2009 to 2018 she was a principal investigator funded by DFG at Universität Bremen, Germany, and from 2013 till 2023 also a project leader in the transregio research unit NAGOCAT, funded by the German Research Foundation (DFG) devoted to a comprehensive study of nanoporous gold as a catalyst. Her group investigates surface reactivity of solids at the atomic level using first-principles quantum-chemical methods, molecular dynamics, statistical theory, microkinetic modelling, and thermodynamics.

REGISTER TO ATTEND

Visit http://bit.ly/3PVDOrf
or scan/click:

science & innovation
Department:
Science and Innovation
REPUBLIC OF SOUTH AFRICA

NRF National Research Foundation

Stellenbosch UNIVERSITY IYUNIVESITHI UNIVERSITEIT