CV and Publications

13 February 2026

Prof. Dr. Lyudmila Moskaleva

Chemistry Department
University of the Free State
PO Box 339, 9300 Bloemfontein, South Africa

Mobile: +27 081 411 0497
Email: moskaleval@ufs.ac.za

Prof. Dr. Lyudmila Moskaleva

University of the Free State, Department of Chemistry
PO Box 339, Bloemfontein 9300, South Africa
Mobile: +27 081 411 0497
Email: moskaleval@ufs.ac.za

13 February 2026

Professor in Physical and Computational Chemistry

Research: Surface reactivity of solids at the atomic and molecular level using first-principles quantum-chemical methods, molecular dynamics, statistical theory, microkinetic modelling and thermodynamics. *Teaching*: Physical Chemistry at undergraduate and Honours levels. *Supervision*: MSc and PhD students, postdocs

Employment

2025 **Full Professor** Chemistry department, University of the Free State, South Africa
2019 **Associate Professor** Chemistry department, University of the Free State, South Africa
2009 **Senior Researcher, Group Leader** Universität Bremen, Germany
2007 Parental leave
2002 **Postdoc, Humboldt Research Fellow,** Department Chemie, TU München, Germany

Education

2001 **PhD Degree** Emory University, USA
1997 **Diploma in Chemistry** Higher Chemical College of the Russian Academy of Sciences at the Mendeleev University of Chemical Technology of Russia, Moscow, Russia

Skills

Research

- Applying suitable levels of theory (DFT, wave-function based methods, QM/MM) to challenging modeling tasks
- Interpretation of data & analysis
- Microkinetic modeling
- AIMD simulations
- Calculation of rate constants from TST and RRKM theory

Engaged Scholarship

- WG3 Co-leader in the COST Action 'COSY'
- Reviewer for NRF, DFG, large HPC centers
- Reviewer for international journals
- Editorial board member for *Scientific Reports*
- Organization of workshops and symposia
- Service on the UFS NRF Rating Committee

Teaching

- Physical Chemistry and Computational Chemistry Courses for BSs and BSc Hons
- Supervision of Postdocs, PhD, Masters, and Honours students
- **External examiner** of 5 PhD and 3 MSc theses by reputed institutions in Germany, South Africa, India, Namibia

Research

- Discovered a new reaction pathway of NOx formation in combustion – via NCN diradical
- Derived from first-principles the rate constants for a number of important combustion reactions – used by researchers worldwide for modeling of combustion processes
- First theoretical study of actinide sorption on a mineral surface (α-alumina) in aqueous environment
- Used quantum-chemical calculations to evaluate accurately important thermodynamic reference data: the heat of formation of uranyl and plutonyl dications
- Applied an advanced cluster embedding method (EPE) to investigate systematically the interaction of coinage metal dimers, trimers, and tetramers with regular sites and O-vacancies on MgO(001)
- Elucidated the mechanism of ethylene to ethylidyne transformation on Pd(111) and Pt(111)
- Elucidated the mechanism of ring opening of a C_5 ring on transition metal surfaces, relevant to HC reforming, fuel upgrading
- Contributed significantly to molecular-level understanding of the catalytic activity of nanoporous gold

Experience in

- Heterogeneous catalysis
- Electrocatalysis
- Organometallic complexes
- Supported metal particles
- Reducible oxides
- Inverse catalysts
- Nanoporous materials
- Hydrocarbon combustion
- Reaction kinetics
- Molecular dynamics

Achievements

- 79 publications in peer reviewed journals, 6 book contributions
- h-index 34, i10-index 62, >3600 citations, 8 articles with >100 citations

Postgraduate Supervision

2022-2025	Cameron Matthews, UFS	Postdoc	Supervisor
2019-2023	Okikiola Olaniyan, UFS	Postdoc	Supervisor
Current	Kgalaletso Otukile, UFS	PhD	Supervisor
2024	Lenard Carroll, UFS	PhD	Supervisor
2023	Shikun Li, Uni Bremen	PhD	Supervisor
2020	Yong Li, Uni Bremen	PhD	Supervisor
2019	Wilke Dononelli, Uni Oldenburg	PhD	Co-Supervisor
2019	Gabriele Tomaschun, Uni Oldenburg	PhD	Co-Supervisor
2009	Zhi-Jian Zhao, TU München	PhD	Co-Supervisor
2009	Shyama Ray, TU München	PhD	Co-Supervisor
2008	Sergey Bosko, TU München	PhD	Co-Supervisor
2008	Mohamed Amjad Basha, TU München	PhD	Co-Supervisor
2006	Kok-Hwa Lim, TU München	PhD	Co-Supervisor
2005	Chan Inntam, TU München	PhD	Co-Supervisor
2024	Sabelo Cele, UFS	MSc	Supervisor
2020	Khanyisile Dhlamini, UFS	MSc	Supervisor
2019	André Wark, Uni Bremen	MSc	Co-supervisor
2015	Gabriele Tomaschun, Uni Oldenburg	MSc	Co-Supervisor
2007	Mathias Winkler, TU München	MSc	Co-Supervisor

Awards

2020 **National Research Foundation of South Africa C1 Rating (Established Researcher),** Pretoria, South Africa

2015 **Best Poster Award, 15th International Congress of Quantum Chemistry**, Beijing, China

2003 **Alexander von Humboldt Foundation Research Fellowship,** Bonn**,** Germany

2000 **Osborn R. Quayle Award for excellence in graduate research,** Department of Chemistry, Emory University, USA

1998 **Osborn R. Quayle Award for excellence in graduate research,** Department of Chemistry, Emory University, USA

International Collaborations and Mobility

- Held research and teaching positions at 4 countries: Russia, USA, Germany, and South Africa
- Past and present collaborations with researchers from 8 countries
- 2021 Working Group 3 co-leader in the EU COST Action COSY
- 2015-2023 Cooperation with leading researchers in Germany within DFG Research Unit NAGOCAT
- 2011-2012 Participation in EU COST Action NANOALLOY

Funding ID

2022 **National research Foundation (NRF), research grant, South Africa/China Joint Science and Technology Research Collaboration,** South Africa, 2022 Grant No: 148775, R 150 000

2021 **National research Foundation (NRF), research grant, South Africa/India Joint Science and Technology Research Collaboration,** South Africa, 2021 Grant No: 133136, R 880 000

2020 **National research Foundation (NRF), NRF Rating, C1,** South Africa, 2020 Grant No: 132047, R 50 000

2018 **German Research Foundation (DFG), research grant, PI in the research unit NAGOCAT,** Germany, 2018 GZ: MO 1863/5, 156 350 EUR

2015 **German Research Foundation (DFG), research grant, PI in the research unit NAGOCAT,** Germany, 2015 GZ: MO 1863/4 and KL 1175/14, 339 200 EUR

2014 **German Research Foundation (DFG), temporary position as a principal investigator,** Germany, 2014 GZ: MO 1863/3, 250 650 EUR

2009 **German Research Foundation (DFG), temporary position as a principal investigator,** Germany, 2009 GZ: MO 1863/2, 230 500 EUR

2007 **German Research Foundation (DFG), research grant with Prof. Notker Rösch,** where I contributed significantly to project conceptualization and realization, Germany, GZ: RO 293/31

2003 **Alexander von Humboldt Foundation**, Alexander von Humboldt Research Fellow, Germany, 2003, 27°600 EUR

Compute Time at National and International HPC Centers

2025 **Centre for High Performance Computing (CHPC),** South Africa, 2020 Research Programme: CHEM1294, 1360 kCore-h (equivalent to 612 000 ZAR)

2024 **Centre for High Performance Computing (CHPC),** South Africa, 2020 Research Programme: CHEM1294, 2304 kCore-h (equivalent to 1 036 700 ZAR)

2023 **Centre for High Performance Computing (CHPC),** South Africa, 2020 Research Programme: CHEM1294, 1278 kCore-h (equivalent to 575 200 ZAR)

2022 **Centre for High Performance Computing (CHPC),** South Africa, 2020 Research Programme: CHEM1294, 2011.5 kCore-h (equivalent to 905 200 ZAR)

2021 **Centre for High Performance Computing (CHPC),** South Africa, 2020 Research Programme: CHEM1294, 643 kCore-h (equivalent to 289 200 ZAR)

2020 **Centre for High Performance Computing (CHPC),** South Africa, 2020 Research Programme: CHEM1294, 281 kCore-h (equivalent to 126 300 ZAR)

2025 **National High-Performance Computing Alliance (NHR),** Germany, 2021 Project No: hbc0061, 4 330 kCore-h (equivalent to 93 820 EUR)

2024 **National High-Performance Computing Alliance (NHR),** Germany, 2021 Project No: hbc0061, 4 420 kCore-h (equivalent to 95 770 EUR)

2023 **National High-Performance Computing Alliance (NHR),** Germany, 2021 Project No: hbc0061, 5 438 kCore-h (equivalent to 117 820 EUR)

2022 **National High-Performance Computing Alliance (NHR),** Germany, 2021 Project No: hbc0061, 5 976 kCore-h (equivalent to 129 480 EUR)

2021 **North-German Supercomputing Alliance (HLRN),** Germany, 2020 Project No: hbc00029, 3 912 kCore-h (equivalent to 84 760 EUR)

2020 **North-German Supercomputing Alliance (HLRN),** Germany, 2019 Project No: hbc00029, 3 528 kCore-h (equivalent to 76 440 EUR)

2019 **North-German Supercomputing Alliance (HLRN),** Germany, 2018 Project No: hbc00029, 2 400 kCore-h (equivalent to 52 000 EUR)

2018 **North-German Supercomputing Alliance (HLRN),** Germany, 2017 Project No: hbc00029, 2 448 kCore-h (equivalent to 53 040 EUR)

2016 **North-German Supercomputing Alliance (HLRN),** Germany, 2015 Project No: hbc00018, 3 600 kCore-h (equivalent to 78 000 EUR)

Selected Invited Talks

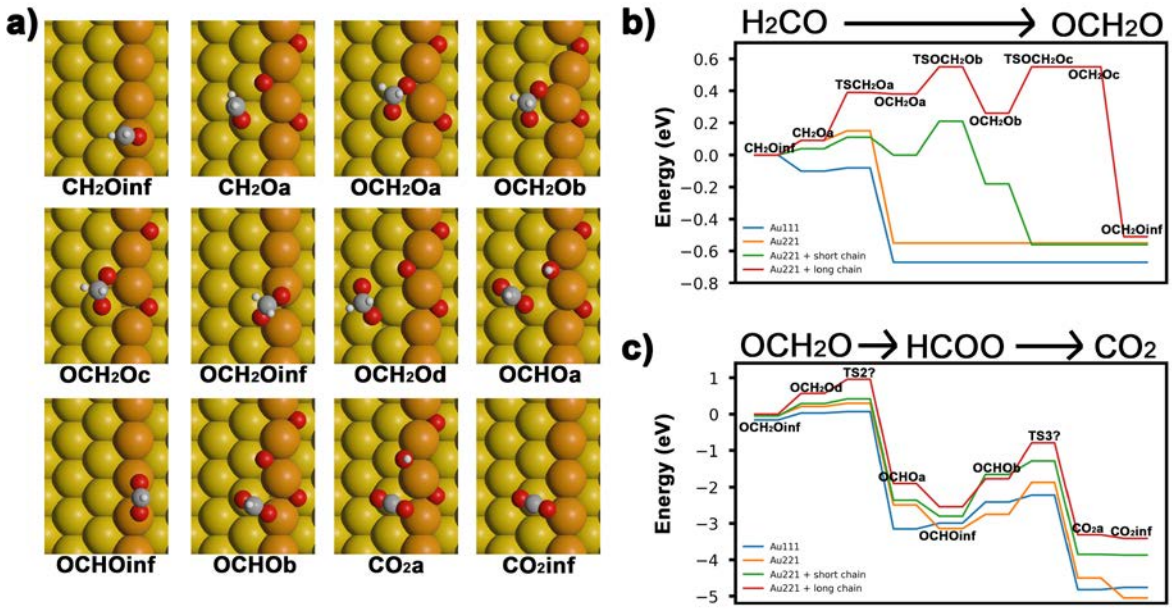
1. *Exploring the Surface Properties and Catalytic Behavior of Nanoporous Gold: A Computational Study*, CATCOSY Workshop, Madrid, Spain, September 26–27, 2024.
2. *Unraveling the Secrets of Nanoporous Gold: A Theoretical Investigation of its Surface Properties and Catalytic Behavior*, Institute for Materials Chemistry, Vienna University of Technology, Vienna, Austria, January 11, 2024.
3. *What Makes Nanoporous Gold a Unique Catalyst? Insights from Modelling Studies of its Surface Chemistry,* NITheCS Colloquium, Stellenbosch, South Africa, November 6, 2023.
4. *Insight into surface chemistry and catalysis on nanoporous gold from modelling studies*, Chem4Energy Annual Conference, Keynote Lecture, Potchefstroom, South Africa, March 29-April 2, 2023.
5. *Formation and catalytic activity of 1D chains of gold oxide from density functional theory*, 32th Annual Conference of the Catalysis Society of South Africa (CATSA), Keynote Lecture, Champagne Sports Resort, Central Drakensberg, South Africa, November 13-16, 2022.
6. *Ab initio molecular dynamics study of the role of oxide-metal interface in catalytic reactions*, COSYES Summer Meeting, Madrid, Spain, June 2-3, 2022.
7. *Computational Studies of Oxidation Catalysis on nanoporous Gold*, Symposium of the Research Unit NAGOCAT, Soderstorf, Germany, May 30-June 1, 2022.

8. *Understanding dioxygen activation on nanoporous gold. A DFT and microkinetic modeling study*, Symposium of the research unit NAGOCAT, Luneburg, Germany, September 9-10, 2019.
9. *Structure and surface chemistry of nanoporous gold: a theoretical study*, Symposium of the Research Unit NAGOCAT, Delmenhorst, Germany, September 28, 2017.
10. *Insights into the catalytic activity of nanoporous gold from a theoretical perspective*, Department of Chemical and Biological Engineering, University of Massachusetts, Amherst, USA, February 23, 2017.
11. *Insights into the surface chemistry of nanoporous gold from theory*, Symposium of the Research Unit NAGOCAT, Delmenhorst, Germany, September 8, 2016.
12. *Metal-oxide interactions studied by a self-consistent QM/MM embedding approach* HeSSSMe ("Helium-mediated Synthesis, Soft-Landing and Spectroscopy of Metal Nanoparticles on Surfaces") Meeting 2014, Madrid, Spain, October 10, 2014.
13. *Silver residues as a possible key to catalytic activity of nanoporous gold: a computational study*, FemEx-Oslo, Oslo, Norway, June 13, 2014.
14. *Nanoporous gold: A low-temperature oxidation catalyst,* A*STAR Institute of High Performance Computing, Singapore, February 18, 2014.
15. *O_2 activation by Ag impurities and CO oxidation on nanoporous gold. A computational study*, HCP-Workshop of the University Oldenburg, Oldenburg, Germany, February 2, 2013.
16. *Gold nanocatalysts promoted by admixtures of silver for low-T CO oxidation and propylene epoxidation*, Institute of Chemistry, University of Oldenburg, Oldenburg, Germany, March 22, 2012.
17. *Role of silver impurities for the catalytic activity of nanoporous gold: a DFT study*, Institute of Theoretical and Computational Chemistry, University of Barcelona, Barcelona, Spain, January 13, 2011.

Research Highlights

1. Partial Oxidation Selectivity in Gold Steered by Low-Coordinated Sites

We collaborated with the experimental team led by the research group at Freie Universität Berlin to analyze their findings on the varying selectivity in the oxidation of methanol to methyl formate on stepped versus flat gold surfaces. An ab initio molecular dynamics (AIMD) simulation was conducted to assess the dynamic evolution of oxygen-covered surfaces. The integration of experimental studies and AIMD simulations revealed that stepped surfaces exhibit greater selectivity towards methyl formate. This is ascribed to the formation of gold-oxygen chains, which reduce the propensity for overoxidation. These insights have significant implications for understanding the catalytic properties of nanoporous gold.



ACS Catalysis

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Letter

Partial Oxidation of Methanol on Gold: How Selectivity Is Steered by Low-Coordinated Sites

Salma Eltayeb, Lenard L. Carroll, Lukas Dippel, Mersad Mostaghimi, Wiebke Riedel, Lyudmila V. Moskaleva,* and Thomas Risse*

Cite This: *ACS Catal.* 2024, 14, 7901–7906

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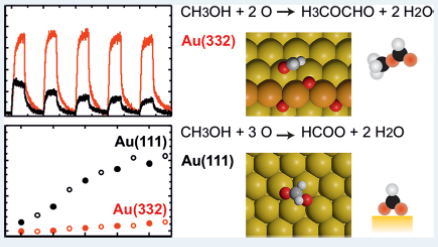
ABSTRACT: Partial methanol oxidation proceeds with high selectivity to methyl formate (MeFo) on nanoporous gold (npAu) catalysts. As low-coordinated sites on npAu were suggested to affect the selectivity, we experimentally investigated their role in the isothermal selectivity for flat Au(111) and stepped Au(332) model surfaces using a molecular beam approach under well-defined conditions. Direct comparison shows that steps enhance desired MeFo formation and lower undesired overoxidation. DFT calculations reveal differences in oxygen distribution that enhance the barriers to overoxidation at steps. Thus, these results provide an atomic-level understanding of factors controlling the complex reaction network on gold catalysts, such as npAu.

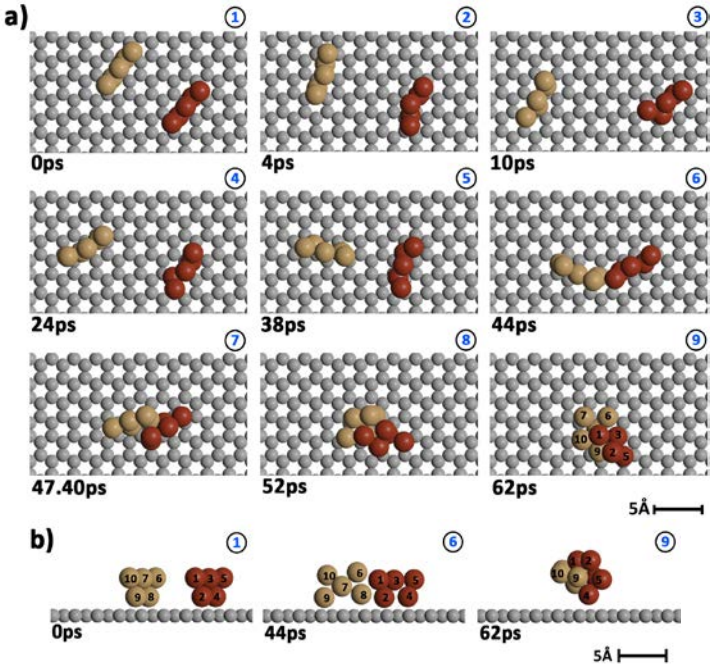


KEYWORDS: *gold, methanol, oxidation, Au(111), Au(332), low-coordinated sites*

S Eltayeb, LL Carroll, L Dippel, M Mostaghimi, W Riedel, LV Moskaleva, T Risse, *ACS Catalysis* 14, **2024**, 7901-7906.

2. Stabilization of subnanometric Cu clusters on graphite and graphene

In this project in collaboration with Dr María Pilar de Lara Castells from CSIC, Madrid, we studied the structural stability of subnanometric Cu_5 clusters on free and defected graphene (a model for HOPG graphite) by means of DFT calculations benchmarked against high-level post-HF approaches, and AIMD simulations at different temperatures.



PCCP

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Cite this: *Phys. Chem. Chem. Phys.*, 2023, **25**, 15729

Carbon vacancy-assisted stabilization of individual Cu_5 clusters on graphene. Insights from *ab initio* molecular dynamics†

Lenard L. Carroll, [a] Lyudmila V. Moskaleva *[a] and María Pilar de Lara-Castells *[b]

Recent advances in synthesis and characterization methods have enabled the controllable fabrication of atomically precise metal clusters (AMCs) of subnanometer size that possess unique physical and chemical properties, yet to be explored. Such AMCs have potential applications in a wide range of fields, from luminescence and sensing to photocatalysis and bioimaging, making them highly desirable for further research. Therefore, there is a need to develop innovative methods to stabilize AMCs upon surface deposition, as their special properties are lost due to sintering into larger nanoparticles. To this end, dispersion-corrected density functional theory (DFT-D3) and *ab initio* molecular dynamics (AIMD) simulations have been employed. Benchmarking against high-level post-Hartree–Fock approaches revealed that the DFT-D3 scheme describes very well the lowest-energy states of clusters of five and ten atoms, Cu_5 and Cu_{10}. AIMD simulations performed at 400 K illustrate how intrinsic defects of graphene sheets, carbon vacancies, are capable of confining individual Cu_5 clusters, thus allowing for their stabilization. Furthermore, AIMD simulations provide evidence on the dimerization of Cu_5 clusters on defect-free graphene, in agreement with the *ab initio* predictions of $(Cu_5)_n$ aggregation in the gas phase. The findings of this study demonstrate the potential of using graphene-based substrates as an effective platform for the stabilization of monodisperse atomically precise Cu_5 clusters.

Received 14th December 2022,
Accepted 7th May 2023

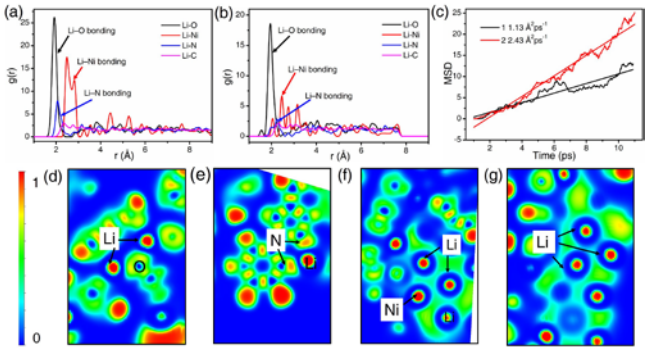
DOI: 10.1039/d2cp05843j

rsc.li/pccp

L Carroll, L Moskaleva, MP de Lara-Castells, *Phys Chem Chem Phys* 25, **2023**, 15729-15743.

3. High-performance anode material for Li-Ion Batteries

This project in collaboration with the experimental work by Wei Shi and Peng Cheng at Nankai University explored coordination compounds as novel anode materials for Li batteries technology. An AIMD simulation at 500 K was carried out to evaluate a dynamic evolution of the structure of Li/anode interface. Experimental mechanistic studies combined with *ab initio* MD simulations showed that the change of structural dimensionality can lead to drastic improvement of the lithium storage performance.



ACS APPLIED MATERIALS & INTERFACES

Research Article

Cite This: ACS Appl. Mater. Interfaces 2019, 11, 25863−25869

www.acsami.org

Formation of One-Dimensional Coordination Chains for High-Performance Anode Materials of Lithium-Ion Batteries via a Bottom-Up Approach

Jia Du,[†,§] Yong Li,[‡,§] Hongwen Liu,[†] Wei Shi,[*,†] Lyudmila V. Moskaleva,[*,‡,¶] and Peng Cheng[*,†]

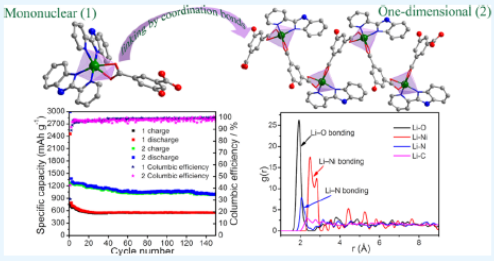
[†]Key Laboratory of Advanced Energy Materials Chemistry (MOE), College of Chemistry, Nankai University, Tianjin 300071, P. R. China

[‡]Institute of Applied and Physical Chemistry and Center for Environmental Research and Sustainable Technology, University Bremen, Bremen 28359, Germany

[¶]Department of Chemistry, University of the Free State, PO Box 339, Bloemfontein 9300, South Africa

Supporting Information

ABSTRACT: Understanding the chemistry of coordination compounds as lithium storage materials is significant for advancing lithium-ion batteries' technology. Coordination compounds have become a new family of versatile anode materials because the metal center, the ligand, and the nonrigid crystal structure can simultaneously contribute to the lithium storage capacity. However, the capacities and cycling abilities of coordination compounds are relatively low in comparison to inorganic nanomaterials, and the mechanism for lithium storage is unclear. This work reports that linking the mononuclear complex $[Ni(PBIM)_2(HIPA)]$ (**1**), where PBIM = 2-(2-pyridyl)benzimidazole, and HIPA = 5-hydroxyisophthalic acid, to a one-dimensional coordination polymer $[Ni(PBIM)(HIPA)]_n$ (**2**) via coordination bonds by a facile bottom-up assembly route can significantly enhance the lithium storage capacity from 554 mA h g^{-1} of **1** to 1025 mA h g^{-1} of **2** at 100 mA g^{-1}. A combined experimental and theoretical study shows that the favorable lithium-ion diffusion pathways afforded by the coordination-chain-based structure of **2** are responsible for its superior electrochemical property.

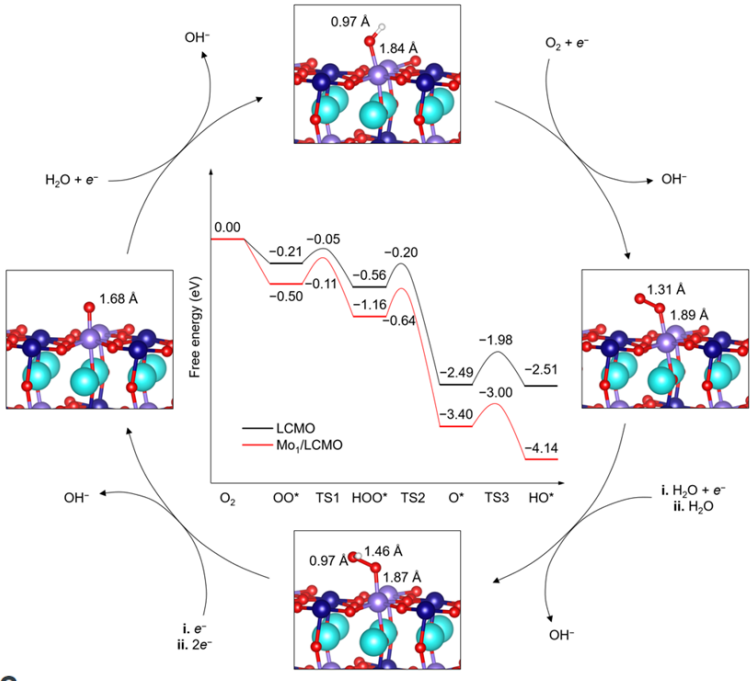


KEYWORDS: *coordination compounds, structural regulation, DFT, AIMD, lithium-ion batteries*

J Du, Y Li, H Liu, W Shi, LV Moskaleva, P Cheng, *Applied Materials & Interfaces* 11, **2019**, 25863-25869.

4. Tuning double perovskite for ORR

The sophisticated computational model included interactions with the solvent and the electrical double layer interface. Our computations demonstrated that dilute electron doping of La_2CoMnO_6 with Mo increases the spin density at Mn sites which expedites the O_2^{2-}/OH^- exchange step. Overall, dilute electron doping leads to a more exothermic reaction pathway and much lower activation barriers for each reaction step explaining the lower overpotential of Mo-doped perovskite toward ORR found in electrochemical experiments.



Energy & Environmental Science

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Cite this: *Energy Environ. Sci.*, 2021, **14**, 1016

Atomically dispersed nonmagnetic electron traps improve oxygen reduction activity of perovskite oxides†

Zechao Zhuang,[a] Yong Li,[b] Yihang Li,[c] Jiazhao Huang,[d] Bin Wei,[e] Rong Sun,[e] Yujing Ren,[f] Jie Ding,[f] Jiexin Zhu,[g] Zhiquan Lang,[h] Lyudmila V. Moskaleva,[b] Chuanxin He,[c] Yu Wang,[i] Zhongchang Wang,[e] Dingsheng Wang *[a] and Yadong Li[a]

Complexity in strongly correlated oxides such as perovskite strictly dominates their performance for oxygen reduction reaction (ORR). Precise control of the physical correlations among spin, charge, orbital, and lattice degrees of freedom in these oxides can exercise considerable enhancement of ORR activity, but has until now remained elusive. Here, we show that nonmagnetic hexavalent molybdenum (Mo^{6+}) atomically dispersed within oxide lattice steers the intrinsic activity of catalytically active sites by entrapping extrinsic electrons at their 3d orbitals, without the occurrence of lattice symmetry breaking and magnetic perturbation. With double perovskite $La_2Co^{2+}Mn^{4+}O_6$ as a model catalyst, the atomic-scale electron trap generates additional high-spin, catalytically active $Mn^{3+}(t_{2g}^3e_g^1)$ sites and highly conductive $Co^{2+}(e_g^2)$–O–$Mn^{3+}(e_g^1)$ double exchange channels, leading to five-fold improvement in ORR activity. First-principles calculations reveal a substantial increase of the spin density on Mn sites caused by electron trapping, and unambiguously confirm a more exothermic reaction pathway as well as a lower barrier of the rate-limiting surface hydroxide regeneration on Mo_1/La_2CoMnO_6. We can also extend this strategy with atomic precision easily to other four oxide catalysts and achieve large enhancement in their ORR activities as anticipated, indicating its broad utility. This work embodies the theories of condensed matter physics in rational design of ORR catalysts, and may inspire further development of the control of electron correlation in strongly correlated electron systems.

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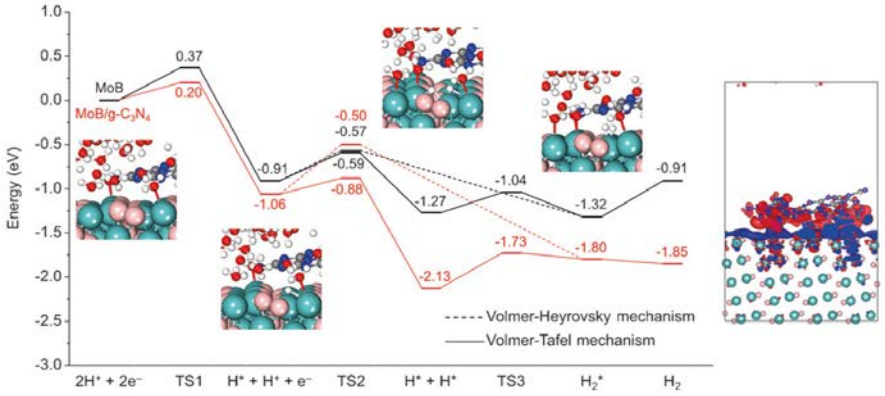
rsc.li/ees

Z Zhuang, Y Li, Y Li, J Huang, B Wei, R Sun, Y Ren, J Ding, J Zhu, Z Lang, LV Moskaleva, C He, Y Wang, Z Wang, D Wang, Y Li, *Energy & Environmental Science* 14, **2021**, 1016-1028.

5. A Schottky catalyst boosts hydrogen evolution

In a collaboration with the group of Prof. Liqiang Mai, Wuhan University of Technology, we reported for the first time a MoB/g-C_3N_4 Schottky catalyst with remarkable HER activity enhancement by inducing the charge redistribution across a Schottky contact with an n-type semiconductor. Computational modelling corroborated vigorous electron transfer from g-C_3N_4 to MoB and showed lowered kinetic barriers of both proton adsorption and reduction on the Schottky catalyst.



GDCh Zuschriften Angewandte Chemie

Electrocatalysis

Deutsche Ausgabe: DOI: 10.1002/ange.201708748
Internationale Ausgabe: DOI: 10.1002/anie.201708748

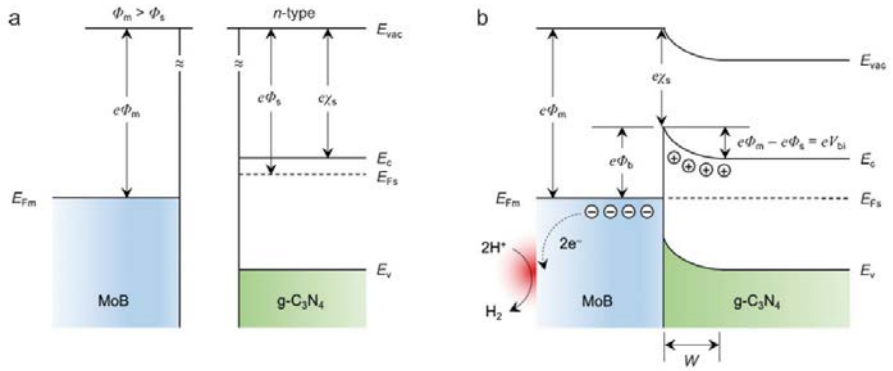
MoB/g-C_3N_4 Interface Materials as a Schottky Catalyst to Boost Hydrogen Evolution

Zechao Zhuang[+], Yong Li[+], Zilan Li[+], Fan Lv, Zhiquan Lang, Kangning Zhao, Liang Zhou, Lyudmila Moskaleva, Shaojun Guo,* and Liqiang Mai**

Abstract: *Proton adsorption on metallic catalysts is a prerequisite for efficient hydrogen evolution reaction (HER). However, tuning proton adsorption without perturbing metallicity remains a challenge. A Schottky catalyst based on metal–semiconductor junction principles is presented. With metallic MoB, the introduction of n-type semiconductive g-C_3N_4 induces a vigorous charge transfer across the MoB/g-C_3N_4 Schottky junction, and increases the local electron density in MoB surface, confirmed by multiple spectroscopic techniques. This Schottky catalyst exhibits a superior HER activity with a low Tafel slope of 46 mV dec^{-1} and a high exchange current density of 17 μA cm^{-2}, which is far better than that of pristine MoB. First-principle calculations reveal that the Schottky contact dramatically lowers the kinetic barriers of both proton adsorption and reduction coordinates, therefore benefiting surface hydrogen generation.*

accepted that further optimization of their catalytic performance lies in more precise tuning of the electron and phonon behaviors.[3,4] Many advances have been reported during the last decade, including creating vacancies,[3c,5] phase transformation,[3b,4a,6] or band engineering,[4b,7] which successfully endow additional active sites to Mo-based catalysts for boosting HER catalysis. However, these tactics often inevitably alter the electron transport property at the same time. In particular, the excessively introduced defects may disorder the primitive lattice and induce the anisotropic scattering of phonons, leading to sharp decreases in electron transport efficiency and loss of activity.[3c,8] Given this, an effective strategy for catalyst surface modulation without perturbing interior conductivity is urgently required.

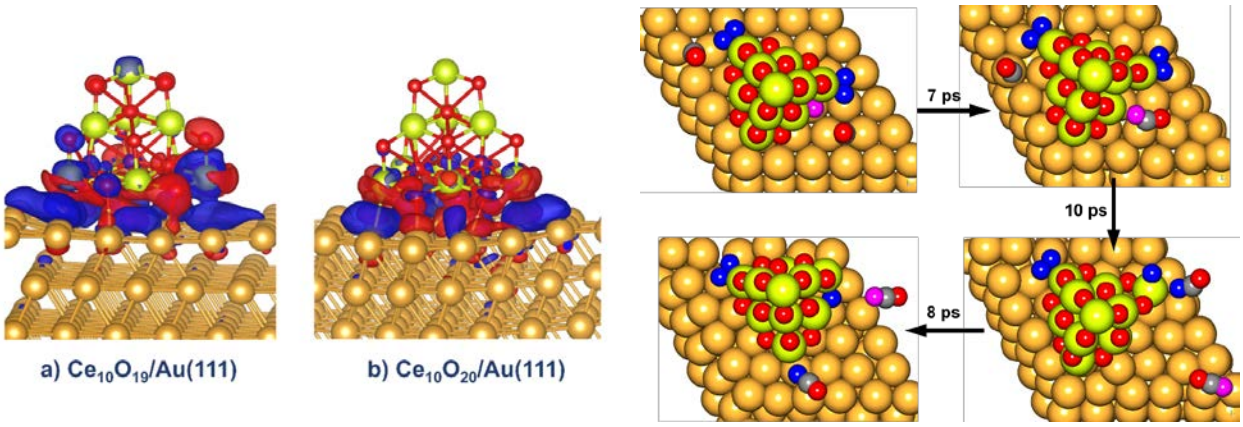
A Schottky junction, formed at the metal–semiconductor interface, is usually introduced to generate the built-in electric



Z Zhuang, Y Li, Z Li, F Lv, Z Lang, K Zhao, L Zhou, L Moskaleva, S Guo, L Mai, *Angewandte Chemie*, 129, **2017**, 1-6.

6. Reactivity of ceria/gold inverse systems

Oxidation reactions catalyzed by Au nanoparticles supported on reducible oxides have been widely studied both experimentally and theoretically, whereas *inverse catalysts*, in which oxide nanoparticles are supported on metal surfaces, received considerably less attention. In both systems the catalytic activity at metal – oxide interfaces can arise not only from each material contributing its functionality, but also from their interactions creating properties beyond the sum of individual components. Inverse catalysts may offer further specific advantages, e.g., the possibility of better control over interfacial sites as well as improved stability, activity, and selectivity. This is the first study addressing the detailed mechanism of CO oxidation on an inverse catalytic system represented by cerium oxide nanoparticles supported on the Au(111) surface by a combination of AIMD simulations and static DFT. A low-energy pathway involving "dual" perimeter sites has been identified theoretically.



a) $Ce_{10}O_{19}$/Au(111) b) $Ce_{10}O_{20}$/Au(111)

ACS Catalysis

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What Changes on the Inverse Catalyst? Insights from CO Oxidation on Au-Supported Ceria Nanoparticles Using Ab Initio Molecular Dynamics

Yong Li, Shikun Li, Marcus Bäumer, Elena A. Ivanova-Shor, and Lyudmila V. Moskaleva*

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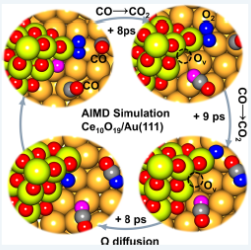
ABSTRACT: Gold-supported ceria nanoparticles (CeO_x/Au), constituting an inverse system with respect to the more commonly studied ceria-supported gold nanoparticles, were previously identified as an excellent catalyst for water–gas shift reaction, CO oxidation, and steam reforming of methanol. However, the electronic structure and reactivity of such inverse catalysts have not been well understood. To probe the inherent nanoparticle–support interactions and their mechanistic role for the catalytic CO oxidation over this composite catalyst, ab initio molecular dynamics simulations and static density functional theory computations have been carried out for Au(111)-supported ceria clusters ($Ce_{10}O_{20/19}$), as a realistic model system of an inverse CeO_x/Au catalyst. We have identified the perimeter of the supported ceria nanoparticle as the most favorable O vacancy formation site; however, the vacancy further migrates to an inner interface site during the thermalization process, simultaneously triggering electron transfer from ceria to Au. Our study shows that the Au(111) surface always withdraws electron density from ceria, irrespective of the chemical environment, namely, in a reducing ($Ce_{10}O_{19}$) as well as oxidizing ($Ce_{10}O_{20}$) environment. To mimic a realistic catalytic environment, CO and O_2 molecules were preadsorbed on the surface of a composite catalyst. We find a vacancy diffusion-assisted Mars–van Krevelen type of reaction mechanism in which the first CO molecule reacts with a lattice O atom of ceria rather than with an activated O_2^{2-} species, forming CO_2 and leaving one O vacancy behind. This vacancy becomes subsequently refilled by an O atom diffusing from the site of O_2 reaction with a second CO molecule, recovering the stoichiometry of the $Ce_{10}O_{19}$ cluster and closing the catalytic cycle. Finally, we discuss differences and similarities between ceria/Au and Au_n/ceria with respect to surface dynamics, charge transfer between the gold and the oxide phases, and the mechanism of CO oxidation.



KEYWORDS: *heterogeneous catalysis, DFT, AIMD simulations, ceria, Au(111) surface, inverse catalyst, CO oxidation, nanoporous gold*

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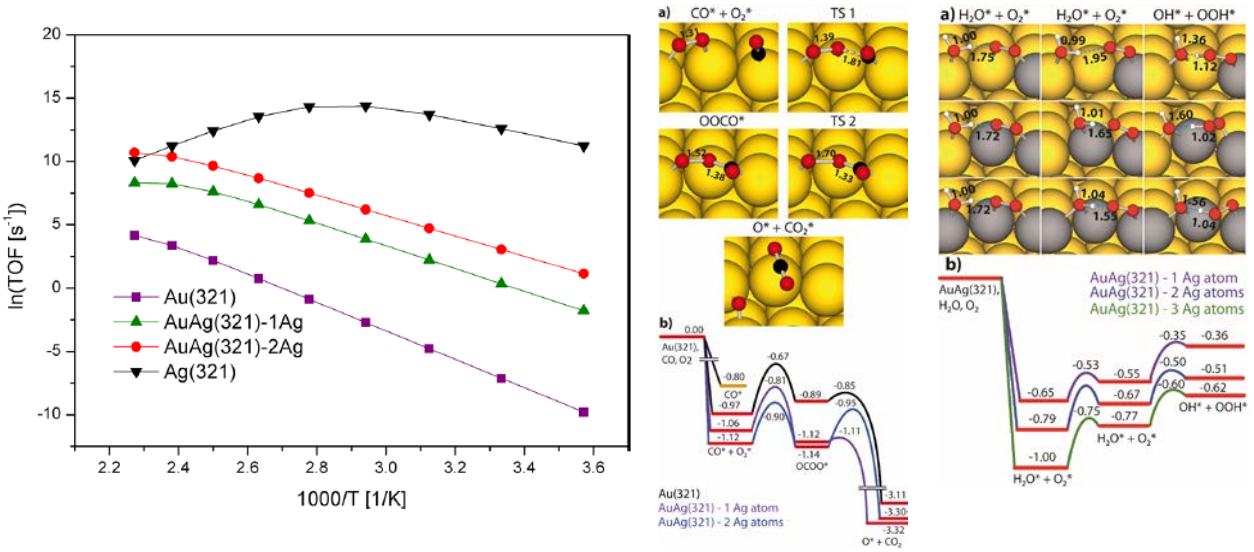
7. Aerobic CO oxidation on nanoporous Au

The splitting of the O-O bond in O_2 has been considered a "bottle-neck" of aerobic gold-based oxidation catalysis. The inability of bulk gold to adsorb and dissociate O_2 is well-known; therefore, the catalytic activity of unsupported np-Au for aerobic oxidation appeared as a surprize and was attributed to residual silver in the np-Au material as a key for its high catalytic activity. Up to now, only a single mechanism, postulating O_2 dissociation, has been assumed in the np-Au community. That mechanism, however, raises concerns because DFT studies consistently predicted rather high activation energies for O_2 dissociation on extended Au surfaces, even if assisted by Ag or another admetal. We presented alternative and energetically more favorable routes for O_2 activation via its direct reaction with CO (a prototype reactant) or water, which act as co-catalyst for O_2 dissociation on np-Au.



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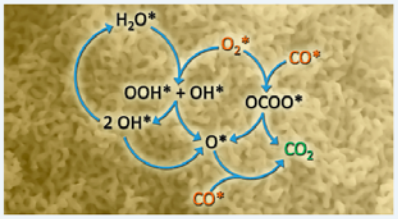
Understanding Oxygen Activation on Nanoporous Gold

Wilke Dononelli,[†] Gabriele Tomaschun,[†] Thorsten Klüner,[†] and Lyudmila V. Moskaleva*[,‡,§]

[†]Institute of Chemistry, Carl von Ossietzky University of Oldenburg, 26129 Oldenburg, Germany
[‡]Department of Chemistry, University of the Free State, PO Box 339, Bloemfontein 9300, South Africa
[§]Institute of Applied and Physical Chemistry and Center for Environmental Research and Sustainable Technology, University of Bremen, 28359 Bremen, Germany

Supporting Information

ABSTRACT: Nanoporous gold (np-Au) is a catalytically highly active material, prepared by selectively dealloying silver from a gold−silver alloy. It can promote aerobic CO oxidation and a range of other oxidation reactions. It has been debated whether the remarkable catalytic properties of np-Au are mainly due to its structural features or whether the residual Ag remaining in the material after dealloying is decisive for the activity, especially for the activation of O_2. Recent theoretical studies provided evidence that Ag impurities can facilitate the adsorption and dissociation of O_2 on np-Au. However, these studies predicted quite a high activation barrier for O_2 dissociation on Au−Ag alloy catalysts, whereas experimentally reported activation energies are much lower. In this work we use the stepped Au(321) surface with Ag impurities, which is arguably a realistic model for np-Au material as well as for Au−Ag catalysts in general. We present alternative routes for O_2 activation via its direct reaction with adsorbed CO or H_2O. In all of the reactions considered, surface atomic O is generated via a sequence of elementary steps with calculated low activation energies of <0.4 eV with respect to coadsorbed reactants. Ag impurities are shown to increase the adsorption energy of O_2 and hence the probability of a surface-mediated reaction versus desorption. We considered four possible mechanisms of CO oxidation in dry and humid environments in a microkinetic modeling study. We show that via the proposed mechanisms water indeed promotes O_2 dissociation; nevertheless, the "dry" mechanism, in which CO directly reacts with O_2, is by far the fastest route of CO_2 formation on pure Au and on Au with Ag impurities. Ag impurities lead to significantly higher turnover rates; thus, calculations point to the key role of Ag in promoting the catalytic activity of Au−Ag alloy systems.

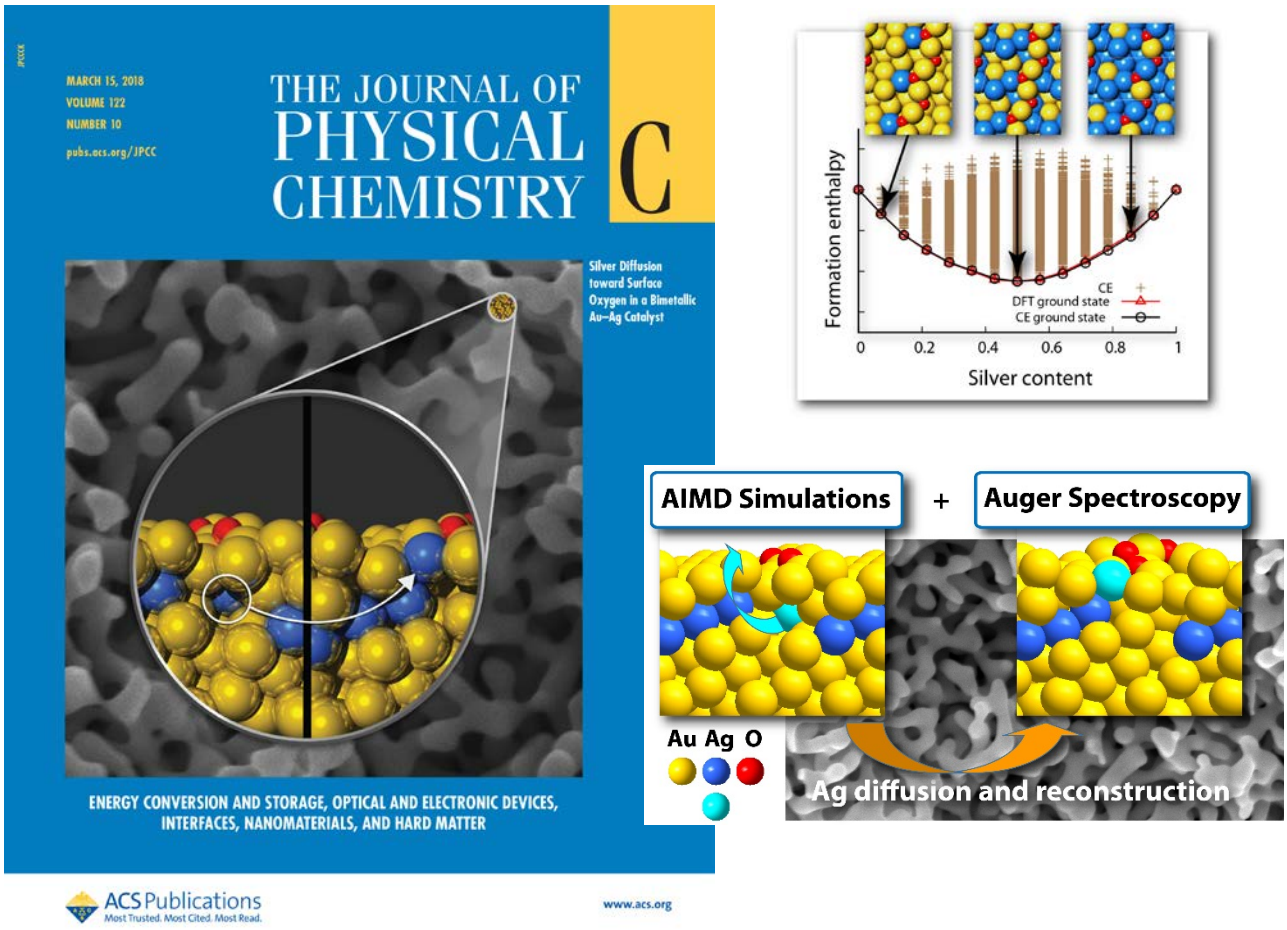


KEYWORDS: *heterogeneous catalysis, gold, nanoporous gold (np-Au), Au(321), oxygen activation, low-coordinated sites, DFT, PBE*

W Dononelli, G Tomaschun, T Klüner, L Moskaleva, *ACS Catalysis*, 9, **2019**, 5204-5216.

8. Oxygen-induced restructuring of Au-Ag alloy surfaces

Several experimental and theoretical studies point towards the role of residual silver in the nanoporous gold material as a key for its high catalytic activity. Hence, knowledge about the distribution of the admetal in the surface region of gold-based alloys is of outmost importance for understanding its role in catalysis. Our theoretical study by means of *ab initio* molecular dynamics (AIMD) combined with an experimental Auger-spectroscopic study found oxygen-driven Ag surface diffusion and the formation of –(O–Au)– chain structures on model surfaces exhibiting structural characteristics of np-Au. As remarkable result, we found that subsurface Ag atoms migrate onto the surface toward oxygen- rich areas and facilitate –(Au–O)– chain formation. Such chains build reservoirs of reactive oxygen, which after having been consumed in chemical reactions would leave behind highly undercoordinated Au atoms, important ingredients to the catalytic activity. We also investigated theoretically the segregation behavior near one-dimensional gold oxide chains on the surface of a catalyst. Such oxide chains seem to display very special properties because the Au-O bonds within them are unusually strong.



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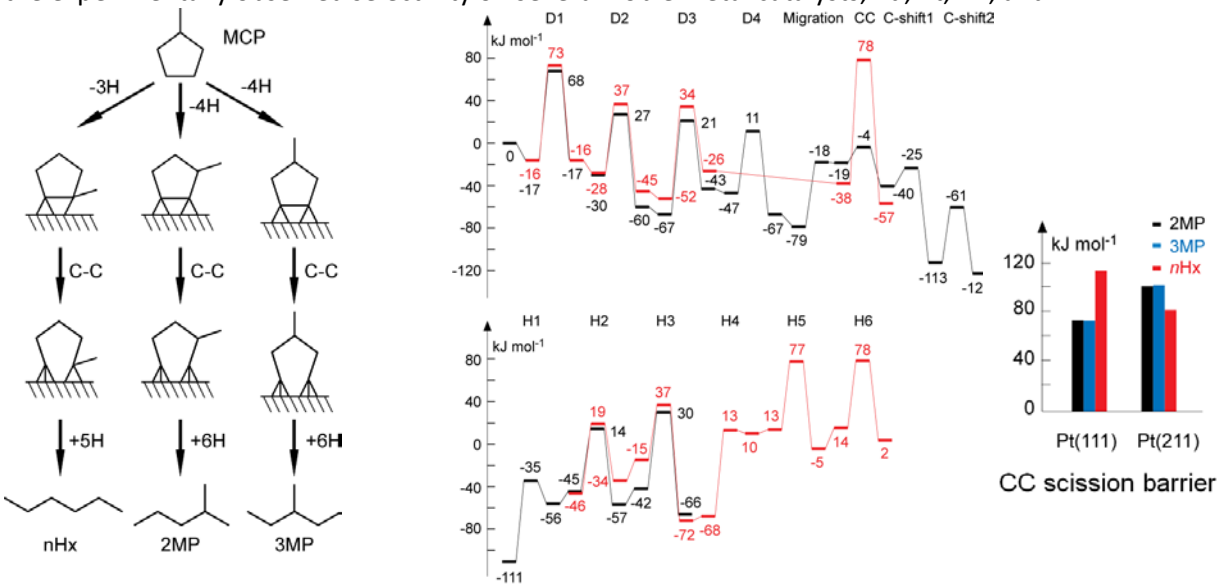
9. Selective C5 ring opening

This theoretical project aimed at clarifying the mechanism of selective ring opening (SRO) of cyclopentane derivatives over supported metal catalysts. Cleavage of C_5 rings is considered to be the crucial step during the conversion of aromatic components of crude oil to hydrocarbons with open-chain structures. We chose methylcyclopentane (MCP) as a model hydrocarbon which is also often used by experimentalists as representative model reaction when studying the catalytic activity and selectivity of SRO. We suggested that the selectivity of MCP ring opening may be different on flat terraces and at steps of metal surfaces. In this way, we were able to rationalize how the selectivity depends on the particle size distribution of a catalyst. In fact, the mechanism of MCP ring opening studied by us eventually allowed us to rationalize the experimentally observed selectivity on several noble metal catalysts, Pd, Pt, Rh, and Ir.



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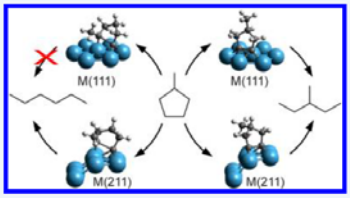
Ring-Opening Reactions of Methylcyclopentane over Metal Catalysts, M = Pt, Rh, Ir, and Pd: A Mechanistic Study from First-Principles Calculations

Zhi-Jian Zhao,[†] Lyudmila V. Moskaleva,[‡] and Notker Rösch*[,†,§]

[†]Department Chemie and Catalysis Research Center, Technische Universität München, 85747 Garching, Germany
[‡]Institut für Angewandte und Physikalische Chemie, Universität Bremen, 28359 Bremen, Germany
[§]Institute of High Performance Computing, Agency of Science, Technology and Research, 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632

Supporting Information

ABSTRACT: Using density functional calculations we studied the conversion of methylcyclopentane to its various ring-opening products, branched and unbranched hexanes, that is, 2-methylpentane and 3-methylpentane, as well as *n*-hexane. We examined four metal catalysts, M = Pt, Rh, Ir, and Pd, using slab models of flat M(111) and stepped M(211) surfaces, to describe terrace-rich large and defect-rich small M particles, respectively. As C−H bond activation and formation is rather independent of the particle structure, we focused on C−C bond scission which is expected to be structure sensitive. The barriers of C−C bond scission indeed vary from ~20 kJ mol^{-1} to ~140 kJ mol^{-1} on various sites of these metal surfaces. In general, lower activation energies were calculated for Rh and Ir surfaces, in agreement with the higher experimental activity of these two metals compared to Pt and Pd. From the calculated C−C bond breaking barriers, we were able to rationalize the selectivity toward different ring-opening products, as observed in experiments over the metal catalysts studied.



KEYWORDS: *ring-opening, methylcyclopentane, reaction mechanism, selectivity, noble metals, DFT calculations*

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