# Rachit Khare | PhD

## Catalysis Research Center, Technical University of Munich

- Chair II for Technical Chemistry (Prof. Dr. Johannes A. Lercher) Technical University of Munich Lichtenbergstraße 4, 85747 Garching (Germany)
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- rachit.khare@tum.de
- rachitkhare.com







"I am interested in combining kinetic and mechanistic studies with operando spectroscopic measurements and theoretical calculations (density functional theory and kinetic modeling) to gain fundamental insights into industrially relevant heterogeneous catalytic systems"

### **EDUCATION**

#### 2011 - 2016Ph.D. in Chemical Engineering

Department of Chemical Engineering & Materials Science University of Minnesota, Minneapolis (USA) Supervised by Prof. Dr. Aditya Bhan

Thesis title: "A Mechanistic Understanding of Light Olefins Selectivity in Methanol-to-Hydrocarbons Conversion on MFI"

#### 2007 - 2011 **B.Tech.** in Chemical Engineering

Department of Chemical Engineering Indian Institute of Technology Roorkee, Roorkee (India)

### **WORK EXPERIENCE**

#### 2021 - present **Group Leader**

Chair of Technical Chemistry II (Prof. Dr. Johannes A. Lercher) Department of Chemistry & Catalysis Research Center Technical University of Munich, Garching (Germany)

Key Research Areas: Heterogeneous Catalysis, X-ray Absorption Spectroscopy, Mechanistic and Kinetic Studies, Density Functional Theory, Electrochemistry, Photochemistry, Data Science in Catalysis

#### 2017 - 2020**Postdoctoral Researcher**

Chair of Technical Chemistry II (Prof. Dr. Johannes A. Lercher) Department of Chemistry & Catalysis Research Center Technical University of Munich, Garching (Germany)

Key Research Areas: Heterogeneous Catalysis, X-ray Absorption Spectroscopy, Catalyst Synthesis and Characterization, Photochemistry

#### 2011 - 2016**Research Assistant**

Department of Chemical Engineering & Materials Science (Prof. Dr. Aditya Bhan) University of Minnesota, Minneapolis (USA)

Key Research Areas: Heterogeneous Catalysis, Mechanistic and Kinetic Studies

#### 2010 Intern

**Panipat Refineries Division** Indian Oil Corporation Limited, Panipat (India)

### **RESEARCH PUBLICATIONS**

2022 Porphyrinic MOF derived single-atom electrocatalyst enables methanol oxidation Z. Zhou, J. Zhang, S. Mukherjee, S. Hou, R. Khare, M. Döblinger, O. Tomanec, M. Otyepka, M. Koch, L. Zhou, W. Li, R.A. Fischer

Chem. Eng. J. doi: 10.1016/j.cej.2022.137888

2022 Highly active and selective sites for propane dehydrogenation in zeolite Ga-BEA L. Ni, R. Khare, R.Bermejo-Deval, R. Zhao, L. Tao, Y. Liu, J.A. Lercher

J. Am. Chem. Soc. doi:10.1021/jacs.2c03810

2022 Speciation of Cu-oxo clusters in FER for selective oxidation of methane to methanol L. Tao, I. Lee, R. Khare, A. Jentys, J. Fulton, M. Sanchez-Sanchez, J.A. Lercher

Chem. Mater. doi:10.1021/acs.chemmater.1c04249

2022 Di- and tetrameric molybdenum sulfide clusters activate and stabilize dihydrogen as

JACS Au doi:10.1021/jacsau.1c00507

‡ eaual contribution

R. Khare<sup>‡</sup>, R. Weindl<sup>‡</sup>, A. Jentys, K. Reuter, H. Shi, and J.A. Lercher

JACS Au 2021 Activity of Cu-Al-oxo extra-framework clusters for selective methane oxidation on Cu doi:10.1021/jacsau.1c00196 exchanged zeolites I. Lee, M.S. Lee, L. Tao, T. Ikuno, R. Khare, A. Jentys, T. Huthwelker, C. Borca, A. Kalinko, O. Gutiérrez, N. Govind, J. Fulton, J.Z. Hu, V.A. Glezakou, R. Rousseau, M. Sanchez-Sanchez, J.A. 2021 Zeolite stabilized di- and tetranuclear molybdenum sulfide clusters form stable Angew. Chem. Int. Ed. doi:10.1002/anie.202015769 catalytic hydrogenation sites <sup>‡</sup> eaual contribution R. Weindl<sup>‡</sup>, R. Khare<sup>‡</sup>, K. Reuter, A. Jentys, H. Shi, J.A. Lercher Featured in the ESRF Research Highlights 2021 2020 Importance of methane chemical potential for its conversion to methanol on Cu-Chem. Eur. J. doi:10.1002/chem.202000772 exchanged mordenite J. Zheng, I. Lee, E. Khramenkova, M. Wang, B. Peng, O. Gutiérrez, J. Fulton, R. Khare, D. Camaioni, A. Jentys, G. Haller, E. Pidko, M. Sanchez-Sanchez, J.A. Lercher Featured on the Front Cover of Chemistry: A European Journal 34/2020 2020 Development of photochemical and electrochemical cells for operando X-ray Phys. Chem. Chem. Phys. absorption spectroscopy during photocatalytic and electrocatalytic reactions doi:10.1039/d0cp00654h R. Khare, A. Jentys, J.A. Lercher 2017 A mechanistic basis for the effect of aluminum content on ethene selectivity in J. Catal. doi:10.1016/j.jcat.2017.02.022 methanol-to-hydrocarbons conversion on HZSM-5 R. Khare, Z. Liu, Y. Han, A. Bhan 2016 Implications of cofeeding acetaldehyde on ethene selectivity in methanol-to-ACS Catal. doi:10.1021/acscatal.5b02818 hydrocarbons conversion on MFI and its mechanistic interpretation R. Khare, S.S. Arora, A. Bhan 2015 Mechanistic studies of methanol-to-hydrocarbons conversion on diffusion-free MFI J. Catal. doi:10.1016/j.jcat.2015.05.012 samples R. Khare, A. Bhan 2015 A mechanistic basis for the effects of crystallite size on light olefin selectivity in J. Catal. doi:10.1016/j.jcat.2014.10.016 methanol-to-hydrocarbons conversion on MFI R. Khare, D. Millar, A. Bhan Featured in the Journal of Catalysis Featured Articles – January 2015 2013 A descriptor for the relative propagation of the aromatics- and olefins-based cycles in J. Catal. doi:10.1016/j.jcat.2013.03.021 methanol-to-hydrocarbons conversion in H-ZSM-5 S. Ilias, R. Khare, A. Malek, A. Bhan 2022 Low-temperature upcycling of polyolefins into liquid alkanes via tandem cracking-Science (under review) W. Zhang, S. Kim, L. Wahl, H. Xu, L. Hale, R. Khare, W. Hu, J. Hu, O.Y. Gutiérrez, Y. Liu, J.A. Lercher 2022 An in-depth study in the confinement of zeolitic Brønsted acid sites by proximal extra-Nat. Catal. (under review) framework Si(OH)<sub>x</sub> groups R. Zhao, R. Khare, Y. Zhang, M. Sanchez-Sanchez, R. Bermejo-Deval, Yue Liu, and J.A. Lercher 2022 Memory transitions in alkali-treated metal organic frameworks controlling the oxygen Energy Environ. Sci. (under review) X. Ma, S. Hou, S. Mukherjee, **R. Khare**, G. Gao, Q. Ai, B. Garlyyev, W. Li, M. Koch, J. Warnan, A.S. Bandarenka, R.A. Fischer **RESEARCH GRANTS AND FUNDING** Danmarks Frie Forskningsfond - Independent Research Fund 2022 Co-proposer (awarded) Spectroscopy of molybdenum sulfide catalysts, from clusters to layers PI: S. Mossin (Denmark Technical University) 2022 Deutsche Forschungsgemeinschaft – Research Grant Co-proposer Low-temperature catalytic upcycling of polyolefin wastes into liquid fuels via tandem (to be submitted) cracking-alkylation: Towards a sustainable refinery PI: J.A. Lercher (Technical University of Munich)

Co-proposer

(in preparation)

2022

**Deutsche Forschungsgemeinschaft – Research Grant** *Olefin dimerization on Ni-exchanged zeolites* 

PI: J.A. Lercher (Technical University of Munich)

Jul 2022 **20th International Zeolite Conference**, Valencia (Spain) Single Ni ions hosted in zeolites as active sites for selective dimerization of butenes **Contributing Author** L. Löbbert, R. Khare, M. Sanchez-Sanchez, J. Lercher Jun 2022 55th German Catalysis Conference, Weimar (Germany) **Presenting Author** Zeolite-encapsulated molybdenum sulfide clusters activate and stabilize hydrogen in the form of hydride species R. Khare, R. Weindl, A. Jentys, J.A. Lercher May 2022 27th North American Catalysis Society Meeting, New York (USA) Hydrothermal stability of Cu-SSZ-39 compared to Cu-SSZ-13 in NH<sub>3</sub>-SCR of NO<sub>x</sub> **Contributing Author** M. Wenig, R. Khare, A. Jentys, J.A. Lercher **Contributing Author** Zeolite encapsulated molybdenum sulfide clusters mimicking the nitrogenase enzyme's active site R. Weindl, R. Khare, H. Shi, J.A. Lercher Mar 2022 33rd German Zeolite Conference, Frankfurt (Germany) Zeolite-encapsulated molybdenum sulfide clusters activate and stabilize hydrogen in the **Presenting Author** form of hydride species R. Khare, R. Weindl, A. Jentys, J.A. Lercher Jan 2022 8th UK Catalysis Conference, Loughborough (England) Nature of active sites in Cu-exchanged small pore zeolites during selective catalytic **Presenting Author** reduction of nitrogen oxides with ammonia R. Khare, M. Wenig, A. Jentys, J.A. Lercher Zeolite stabilized molybdenum sulfide clusters activate hydrogen as hydride species and **Contributing Author** form stable catalytic hydrogenation sites R. Weindl, R. Khare, A. Jentys, J.A. Lercher Jan 2021 European XFEL and DESY User Meeting (Online) **Presenting Author** Development of operando reaction cell for simultaneous measurement of UV-Vis DRS and XAS at P64/65 R. Khare, A. Jentys, J.A. Lercher Dec 2020 Conference on Operando Characterization of Catalysts at Work (Online) Monitoring the dynamic nature of active sites in Cu-exchanged zeolites during selective **Presenting Author** catalytic reduction of NO<sub>x</sub> using operando X-ray absorption spectroscopy R. Khare, M. Wenig, A. Jentys, and J.A. Lercher Awarded best oral presentation Jun 2020 17th International Congress on Catalysis, San Diego (USA) Nature of active sites in Cu/AEI during selective catalytic reduction of NO<sub>x</sub> with NH₃ using **Presenting Author** operando X-ray absorption spectroscopy R. Khare, M. Wenig, R.B. de Val, A. Jentys, J.A. Lercher Feb 2020 ESRF User Meeting, Grenoble (France) Monitoring structural changes in Mo<sub>x</sub>S<sub>v</sub> phase encaged within the confinement of zeolites **Presenting Author** via HERFD-XAS and VtC-XES measured under sulfidation/hydrogenation conditions R. Khare, R. Weindl, H. Shi, A. Jentys, J.A. Lercher Jan 2020 European XFEL and DESY User Meeting, Hamburg (Germany) Nature of Cu active species in small pore zeolites during NH<sub>3</sub>-SCR **Presenting Author** R. Khare, A. Jentys, J.A. Lercher Dec 2019 EBS Workshop on X-ray Emission Spectroscopy, Grenoble (France) **Presenting Author** Monitoring structural changes in Mo<sub>x</sub>S<sub>V</sub> phase encaged within the confinement of zeolites via HERFD-XAS and VtC-XES measured under sulfidation/hydrogenation conditions R. Khare, R. Weindl, H. Shi, A. Jentys, J.A. Lercher Jul 2016 16th International Congress on Catalysis, Beijing (China) Catalytic consequences of the dual aromatics- and olefins-based cycles on light olefin **Contributing Author** selectivity in methanol to hydrocarbons conversion R. Khare, A. Hwang, A. Bhan 251st American Chemical Society National Meeting, San Diego (USA) Mar 2016 Enhancing light olefin selectivity in methanol-to-hydrocarbons conversion by cofeeding **Presenting Author** oxvaenates R. Khare, S.S. Arora, A. Bhan Dec 2015 International Chemical Congress of Pacific Basin Societies, Honolulu (USA)

Zeolites with nanometer diffusion lengths: Mechanistic implications in shape selective catalytic conversion of methanol to hydrocarbons

Contributing Author

D. Millar, R. Khare, A. Bhan

Jun 2015 24th North American Catalysis Society Meeting, Pittsburgh (USA)

A mechanistic basis for the effects of crystallite size on light olefin selectivity in methanolto-hydrocarbons conversion on MFI

**Presenting Author** 

**Presenting Author** 

**Presenting Author** 

**Presenting Author** 

R. Khare, D. Millar, A. Bhan

Nov 2014 American Institute of Chemical Engineers Annual Meeting, Atlanta (USA)

A mechanistic basis for the effects of crystallite size on light olefin selectivity in methanol-

to-hydrocarbons conversion on MFI R. Khare, D. Millar, A. Bhan

Nov 2013 American Institute of Chemical Engineers Annual Meeting, San Francisco (USA)

Kinetics and mechanisms of aromatic methylation and dealkylation in methanol-to
Contributing Author

hydrocarbons conversion on HZSM-5: What are the aromatics precursors to light olefins?

S. Ilias, I.M. Hill, R. Khare, A. Bhan

Dec 2009 8th Indo-German Winter Academy, Roorkee (India)

Combined thermal and solar power generation. What does it bring for the future?

R. Khare

Sep 2009 Students' Congress of Indian Institute of Chemical Engineers, Roorkee (India)

Arsenic removal from drinking water using electrocoagulation and optimization of its

parameters using response surface methodology

R. Khare, S. Sharma, A. Kumar, I.M. Mishra

**POSTERS** 

May 2022 27th North American Catalysis Society Meeting, New York (USA)

Nature of active sites in Cu-exchanged small pore zeolites during NH<sub>3</sub>-SCR: an operando X- Contributing Author

ray absorption spectroscopy study

R. Khare, M. Wenig, A. Jentys, J.A. Lercher

Mar 2021 **54th German Catalysis Conference**, Weimar (Germany)

Effect of Ni loading and Brønsted acidity on the performance of FAU zeolites in butene Contributing Author

dimerization

L. Löbbert, R. Khare, R.B. deVal, M. Sanchez-Sanchez, J.A. Lercher

Mar 2020 **53rd German Catalysis Conference**, Weimar (Germany)

A mechanistic study of selective partial photo-oxidation of primary and secondary

alcohols to aldehydes and ketones under visible light illumination on graphitic carbon

nitride

R. Khare, A. Jentys, J.A. Lercher

R. Khare, A. Jentys, J.A. Lercher

Mar 2019 **52nd German Catalysis Conference**, Weimar (Germany)

Selective partial oxidation of  $C_1$ - $C_3$  alcohols to aldehydes/ketones on graphitic carbon

Presenting Author

nitride under visible light illumination

Mar 2016 **251st American Chemical Society National Meeting**, San Diego (USA)

Enhancing light olefin selectivity in methanol-to-hydrocarbons conversion by co-feeding Presenting Author

oxygenates

R. Khare, S.S. Arora, A. Bhan

Aug 2015 Gordon Research Conference on Nanoporous Materials, Holderness (USA)

Methanol-to-hydrocarbons conversion: Effects of crystallite size and intrinsic mechanistic

Presenting Author

behavior of MFI

R. Khare, D. Millar, A. Bhan

Aug 2015 Gordon Research Seminar on Nanoporous Materials, Holderness (USA)

Methanol-to-hydrocarbons conversion: Effects of crystallite size and intrinsic mechanistic Presenting Author

behavior of MFI

R. Khare, D. Millar, A. Bhan

Aug 2014 Gordon Research Conference on Catalysis, New London (USA)

A mechanistic basis for the effects of crystallite size on light olefin selectivity in methanol-

to-hydrocarbons conversion on MFI

R. Khare, D. Millar, A. Bhan

AWARDS AND HONORS			
2020	Best Oral Presentation Award Conference on Operando Characterization of Catalysts at Work		
2015	Doctoral Dissertation Fellowship University of Minnesota, Minneapolis (USA)	\$22000	
2011	Best Thesis Award (B.Tech. Chemical Engineering) Indian Institute of Technology Roorkee, Roorkee (India)		
2007	University Scholarship Indian Institute of Technology Roorkee, Roorkee (India)	1 year tuition fee	
TEACHING			
2022	Industrial Chemical Processes II M.Sc., Department of Chemistry, Technical University of Munich	Lecturer	
2022	Methods of Catalysis M.Sc., Department of Chemistry, Technical University of Munich	Lecturer	
2021	Methods of Catalysis M.Sc., Department of Chemistry, Technical University of Munich	Lecturer	
2019	Technical Chemistry Praktikum  B.Sc., Department of Chemistry, Technical University of Munich	Lab Supervisor	
2018	Technical Chemistry Praktikum  B.Sc., Department of Chemistry, Technical University of Munich	Lab Supervisor	
2017	Technical Chemistry Praktikum  B.Sc., Department of Chemistry, Technical University of Munich	Lab Supervisor	
2014	Physical and Chemical Thermodynamics  B.ChEn., Department of Chemical Engineering & Materials Science, University of Minnesota	Teaching Assistant	
2014	Chemical Engineering Design B.ChEn., Department of Chemical Engineering & Materials Science, University of Minnesota	Teaching Assistant	
2012	Reaction Kinetics and Reactor Design B.ChEn., Department of Chemical Engineering & Materials Science, University of Minnesota	Teaching Assistant	
STUDENT SUPERVISION			
2022	Heewoo Seo, Department of Chemistry, TU Munich Photochemical reduction of carbon dioxide to methanol	M.Sc. Internship (on-going)	
2022	<b>Disha Malik</b> , Department of Chemical Engineering, Delhi Technological University <i>X-ray absorption/emission spectroscopy study of 3d-transition metals on bench-top easyXAFS</i> Funded by: Deutscher Akademischer Austauschdient (DAAD)	B.Tech. Internship	
2020	Angelica Tessa Yunanto, Department of Chemical Engineering, TU Munich Photocatalytic hydrogen evolution reaction on graphitic carbon nitride	M.Sc. Internship	
2020	<b>Xhang Xiaoyang</b> , Department of Chemical Engineering, TU Munich Electrocatalytic reduction of carbon dioxide	M.Sc. Internship	
2019	Valentin Menzel, Department of Chemistry, TU Munich Electrocatalytic conversion of carbon dioxide to methanol	M.Sc. Thesis	
2019	Corbinian grön, department of chemistry, tu munich Partial alcohol oxidation under visible light illumination	B.Sc. Thesis	
2019	Daphne Bondal, Department of Chemistry, TU Munich Carbon dioxide hydrogenation to carbon dioxide	B.Sc. Thesis	
2019	<b>Marcus Chua Wen Hao</b> , Department of Chemistry, TU Munich Synthesis and characterization of novel catalysts for photocatalytic and electrocatalytic $CO_2$ reduction	B.Sc. Thesis	
2019	<b>Dominik Grünwald</b> , Department of Chemistry, TU Munich Selective oxidation of alcohols with simultaneous evolution of $H_2$ by $g-C_3N_4$ under visible light illumination	B.Sc. Thesis	

illumination

2019	Faishal Inshauddin, Department of Chemistry, TU Munich Photocatalytic conversion of carbon dioxide to fuels	B.Sc. Thesis
2018	<b>Matthias Schmidt</b> , Department of Chemical Engineering, TU Munich Chemical methanation of CO <sub>2</sub> as a catalytic Process	M.Sc. Internship
2018	Angelica Tessa Yunanto, Department of Chemical Engineering, TU Munich Electrocatalytic hydrogen evolution reaction and reduction of carbon dioxide	B.Sc. Thesis
2018	<b>Peggy Jing-Ting Huang</b> , Department of Chemical Engineering, TU Munich Photocatalytic hydrogen evolution on $Pt/g-C_3N_4$ under visible light illumination	B.Sc. Thesis
2018	Magdalena Maria Kleybolte, Department of Chemistry, TU Munich Photocatalytic hydrogen evolution graphitic carbon nitride	B.Sc. Thesis
2018	<b>Ernest Jian Ming Yap</b> , Department of Chemistry, TU Munich <i>Photochemical conversion of carbon dioxide on g-C</i> <sub>3</sub> N <sub>4</sub> <i>catalysts</i>	B.Sc. Thesis
2018	Zhen Yu Choong, Department of Chemistry, TU Munich Catalytic conversion of carbon dioxide to methanol	B.Sc. Thesis
2018	<b>Stephen Liefeldt</b> , Department of Chemistry, TU Munich Synthesis of single atom bimetallic alloys supported on $g$ - $C_3N_4$	B.Sc. Thesis
EXPER	IENCE AT X-RAY SYNCHROTRON FACILITIES	
Aug 2	P65 <b>German Electron Synchrotron DESY</b> , Hamburg (Germany), <b>120 hours</b> Low temperature upcycling of polyolefins in Lewis acidic ionic liquids: Effect of metal additives	<b>Co-proposer</b> (accepted)
Jul 2	Balder <b>MAX IV</b> , Lund (Sweden), <b>120 hours</b> Elucidating the electronic and structural properties of Fe-, Co-, or Ni-promoted Mo sulfide clusters encapsulated within the micropores of NaY zeolite	Co-proposer (accepted)
May 2	Phoenix <b>Swiss Light Source</b> , Villigen (Switzerland), <b>120 hours</b> Upcycling of polyolefins in Lewis acidic ionic liquids: Elucidation of key ion pairing interactions	Co-proposer
Apr 2	1D26 European Synchrotron Radiation Facility, Grenoble (France), 96 hours  Understanding the effects of electronic properties of Ni in zeolites and metal organic frameworks on its activity for butene dimerization	Co-proposer
Nov 2	P64 <b>German Electron Synchrotron DESY</b> , Hamburg (Germany), <b>96 hours</b> Understanding the effects of electronic structure of Pt on hydrogen adsorption from aqueous phase during electrocatalytic hydrogenation	Co-proposer
Sep 2	D21 ID26 European Synchrotron Radiation Facility, Grenoble (France), 144 hours  Elucidating the structural similarities between Fe-Mo sulfide clusters encapsulated in the micropores of NaY zeolite and the FeMo-cofactor of the nitrogenase enzyme	Co-proposer
Aug 2	P65 <b>German Electron Synchrotron DESY</b> , Hamburg (Germany), <b>144 hours</b> Elucidating the structure of Fe-Mo sulfide clusters encapsulated in zeolite NaY during hydrogenation catalysis	Co-proposer
May 2	P64 <b>German Electron Synchrotron DESY</b> , Hamburg (Germany), <b>118 hours</b> The nature of active sites in Cu/CHA and Cu/AEI during $NH_3$ -SCR of $NO_x$ : A study using spatially resolved operando Cu KB-VtC X-ray emission spectroscopy	Co-proposer
2018–2	P65 <b>German Electron Synchrotron DESY</b> , Hamburg (Germany), <b>522 hours</b> Operando studies on photo-(electro-)catalysts under dynamic reaction conditions	Co-proposer
Nov 2	Phoenix <b>Swiss Light Source</b> , Villigen (Switzerland), <b>120 hours</b> Linking structural changes in small-pore zeolites with the nature of Cu-species during the selective catalytic reduction of NO <sub>x</sub> with NH <sub>3</sub>	Co-proposer
Jul 2	P65 <b>German Electron Synchrotron DESY</b> , Hamburg (Germany), <b>96 hours</b> Photo/electro-catalytic conversion of carbon dioxide to methanol on Rh@Au single-atom bimetallic alloys	Co-proposer
Nov 2	Phoenix <b>Swiss Light Source</b> , Villigen (Switzerland), <b>72 hours</b> The structure of copper ions coordinated to Al T-sites during methane oxidation: Al XAFS, Cu L-edge XANES and TDDFT-based XANES calculations	Participant

Oct 2018 ID26 European Synchrotron Radiation Facility, Grenoble (France), 120 hours Participant, Organizer Monitoring structural evolution during sulfidation and catalysis of dispersed Ni-Mo(W) phase within three-dimensional confines via in situ XAS P64 German Electron Synchrotron DESY, Hamburg (Germany), 118 hours Sep 2018 Co-proposer Formation of copper oxo clusters in zeolites for the selective oxidation of methane to methanol at low temperature 2017-2018 P65 German Electron Synchrotron DESY, Hamburg (Germany), 558 hours Participant, Organizer Operando studies on catalysts under dynamic conditions BM26A European Synchrotron Radiation Facility, Grenoble (France), 144 hours Sep 2017 Participant, Organizer Determining the structure, concentration and intrinsic activity of Ni-promoted sites in Ni-Mo-W sulfide catalysts via in situ and operando studies P65 German Electron Synchrotron DESY, Hamburg (Germany), 120 hours **Participant** Dec 2016 In situ investigations of the active state of Rh Co-catalysts on semiconductors during photocatalytic H<sub>2</sub> production via overall water splitting

### SKILLS

**Programming** Python · Matlab · SQL

**Quantum Chemistry Packages** Orca · Quantum Espresso · CP2K · NWChem

**Database Management Tools** 

### PROFESSIONAL ACTIVITIES

**Reviewed Journals** Journal of Catalysis

**ACS Catalysis** 

Applied Catalysis A: General Applied Catalysis B: Environmental

Industrial & Engineering Chemistry Research Microporous and Mesoporous Materials

**Catalysis Communications** 

**Reviewed Conferences** North American Catalysis Society Meeting

### **REFERENCES**

Prof. Dr. Johannes A. Lercher Professor (Chair of Technical Chemistry II) Department of Chemistry & Catalysis Research Center <u>johannes.lercher@ch.tum.de</u> Technical University of Munich **L** +49 89 289 13544 Garching, Germany

**Group page**

Prof. Dr. Aditya Bhan Professor

 <u>abhan@umn.edu</u> Department of Chemical Engineering & Materials Science University of Minnesota **L** +1 612 626 3981 Minneapolis, USA

Group page

Prof. Dr. Karsten Reuter Director

> Theory Department <u>reuter@fhi.mpq.de</u>

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