Nicholas Ryan Jaegers

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EDUCATION

PhD Chemical Engineering — *Washington State University*
December 2019 — Pullman, Washington
Advisor: Prof. Yong Wang

BS Chemical Engineering, Nuclear Engineering Minor, University Honors Program, Cum Laude — *Iowa State University*
May 2014 — Ames, Iowa

ACADEMIC AND RESEARCH APPOINTMENTS

University of New Mexico; Albuquerque, NM
January 2025 – Present — **Assistant Professor**

University of California, Berkeley; Berkeley, CA
July 2020 – January 2025 — **Postdoctoral Scholar** – Supervisor: Prof. Enrique Iglesia

- *Assessed selective oxidation, dehydrogenation, hydrogenation, and dimerization pathways for metal oxides using kinetic, spectroscopic, computational, and transient approaches*
- *Collaboratively worked and communicated with industry sponsors at ExxonMobil and BASF*
- *Maintained and improved group computing, IT, and safety systems*

Pacific Northwest National Laboratory; Richland, Washington
February 2020 – June 2020 — **Post Doctorate Research Associate C** – Supervisor: Dr. Jian Zhi Hu
July 2016 – January 2020 — **PhD Intern – Catalysis** – Supervisor: Dr. Jian Zhi Hu
September 2015 – July 2016 — **Alternate Sponsored Fellow** – Mentor: Dr. Jian Zhi Hu

- *Developed and exploited new in-situ HTHP MAS NMR spectroscopy methods*
- *Identified active catalytic structures of transition metal oxides using a DFT-aided NMR approach*
- *Synthesized, characterized, and tested of metals and oxide materials with well-defined structures*
- *Deciphered solvation structures of next-generation electrolyte solutions for energy storage applications*
- *Identified toxic by-products of low-temperature ENDS via MAS NMR*
- *Collaboratively worked in a multi-disciplinary environment with many institutions around the globe*

Washington State University; Pullman, Washington
January 2015 – July 2016 — **Research Assistant** – Advisor: Prof. Yong Wang

- *Probed catalytic systems for heterogeneously catalyzed methanol carbonylation using in-situ IR spectroscopy*

Center for Sustainable Environmental Technologies, Biorenewables Research Laboratory; Ames, Iowa
January – May 2013 — **Research Assistant** – Supervisor: Patrick Johnston

- *Prepared samples and ran experimental procedures for thermochemical conversion of biomass via micropyrolysis*

Iowa State University; Ames, Iowa
August – December 2012 — **Honors Research Project** – Mentor: Dr. Robert Brown
January – May 2010 — **Honors Mentor Program** – Mentor: Dr. Young-Jin Lee

- *Investigated impact of corn stover phenotypes on bio-oil components using micro-pyrolysis for grant claim*
- *Investigated mass spectrometry techniques for evaluation of algae-based biofuel*

COURSE INSTRUCTION

Thermodynamics
CBE 302: S25, S26
Department Seminar
CBE 501; BME 567, NSME 595: S25, F25
Catalysis Seminar
CBE 403/503: S26

Process Controls
CHE 411: F14 (Teaching Assistant, WSU)

INDUSTRIAL EXPERIENCE

Nanode Battery Technologies, Ltd.
June 2021 – January 2022 **Consultant** – Berkeley Science Fellows Program
- *Provided recommendations and scientific advice on electrolyte-electrode interactions for next-generation batteries*
- *Conducted computational simulations of electrode surfaces*

Alliant Energy Co.; Madison, Wisconsin
May – August 2014 **Performance & Planning Intern** – Supervisor: Andrew Szafarz
- *Assessed SCR technologies and assisted emissions system installation efforts for coal-fired generating stations*
- *Conducted heat survey in coal-fired generating station*

International Paper: Cedar River Mill; Cedar Rapids, Iowa
June 2013 – January 2014 **Process Engineer Intern** – Supervisor: Tim Berg
- *Developed real-time operational metrics tool dashboard for plant function*
- *Conducted ongoing safety-related experiments and communicated data and recommendations*
- *Analyzed and monitored process metrics for quality, reliability, and consistency*
- *Conducted process improvement testing on alternative chemicals and operating parameters*

Iowa DNR on assignment with Green Plains Renewable Energy; Lakota, Iowa
May – August 2012 **Pollution Prevention Intern** – Supervisor: Matt Millage
- *Monitored ongoing water usage and allocation at 112 MMGY ethanol plant*
- *Proposed operational changes to realize a 79 MMGY (~30%) reduction in water usage (51 MMGY instituted)*
- *Drafted proposal for decreased chemical usage and power savings to decrease emissions by 330 tons CO_2/year*

AWARDS AND SHOLARSHIPS

2024: ACCESS Research Allocation ($3000)
2023: Pines' Academic Laboratory Management and Leadership Symposium (sponsored), Global NMR Twitter Conference (second prize)
2021: XSEDE Research Allocation ($8,000), ACS Postdoc to Faculty Workshop
2020: PNNL Outstanding Performance Award, PNNL Outstanding Performance Award – Significant Service, International Congress on Catalysis Travel Award, International Congress on Catalysis Young Scientist Presenter Award, NERSC Exploratory Allocation, XSEDE Startup Allocation
2019: North American Catalysis Society Kokes Award, PI for PNNL FY19 Quickstarter Proposal "Formulating Cooler Butenes," PNNL Outstanding Performance Award
2018: PI for PNNL FY18 Quickstarter Proposal "Pathway to Cooler Chemicals," Alaska Airlines Imagine Tomorrow Travel Award
2017: AIChE Catalysis and Reaction Engineering Division Travel Award
2014 – 2017: Achievement Rewards for College Scientists Fellowship
2013: Black & Veatch Building a World of Difference Renewable Energy Scholarship, Nicholas L. Reding/Monsanto Scholarship in Engineering, Omaha Public Power District Nuclear Engineering Scholarship
2012: Fahrney Education Foundation Scholarship, Academic Recognition Award, Roderick Seward, Flossie Scholarship, Ratcliffe & Helen M. Galloway Scholarship
2011: Fahrney Education Foundation Scholarship, Academic Recognition Award, Frederick Martinson Scholarship
2010: Fahrney Education Foundation Scholarship, Academic Recognition Award, Robert C. Byrd Honors Scholarship, Don Delahunt Award, Kenneth & Mary Heilman Award, Iowa Grocers Education Foundation Scholarship
2009: Fahrney Education Foundation Scholarship, Academic Recognition Award, Robert C. Byrd Honors Scholarship, Elks National Foundation Scholarship, Grand Masonic Lodge of Iowa Scholarship, National FFA Organization Iowa Scholarship, Cargill Community Scholarship

SERVICE AND AFFILIATIONS

Rocky Mountain Catalysis Society (Treasurer, 2025 – Present)
Conference Organizer: Global NMR Online Conference 2024
Conference Session Chair: NAM28: "Structure-Activity Relations", ACS 2022: "Materials for Energy & Catalytic Applications", LSAC Symposium, NAM29: "C_2-C_{3+} Hydrocarbons C-C coupling, Isomerization and Cracking Reactions"
American Institute of Chemical Engineers (Columbia Valley Section Secretary, 2016 – 2020)

Meeting Reviewer: 18th International Congress on Catalysis, 17th International Congress on Catalysis, 4th International Electronic Conference on Applied Sciences
Grant Reviewer: ACS Petroleum Research Fund, Stanford Synchrotron Radiation Lightsource
Journal Reviewer: *Applied Catalysis B*, *Journal of Catalysis*, *ACS Catalysis, ACS Omega*, *Catalysis Today, scientific reports, Reaction Chemistry and Engineering, International Journal of Environmental Research and Public Health*, *Journal of Environmental Chemical Engineering, batteries*, *ChemEngineering*, *chemosensors*, M*olecules, nanomaterials, nanomanufacturing, recycling, sustainability, Water, Symmetry*
Editorial Duties: Special Issue *Inorganics*, *Molecules* Early Career Editorial Board
American Chemical Society
National Eagle Scout Association
Order of the Arrow: Lodge Service Award, Jim Gooding Award, Vigil Honor Membership

PUBLICATIONS

2025

1. Mikalai A. Artsiusheuski, Nicholas R. Jaegers, Carlos Lizandara Pueyo, and Enrique Iglesia **Selective ethylbenzene dehydrogenation to styrene at Lewis acid-base pairs on zirconia surfaces** *ACS Catalysis* 2025 DOI: 10.1021/acscatal.5c04904

2. Nicholas R. Jaegers, Miroslaw A. Derewinski, Eric D. Walter, Iskra Z. Koleva, Daria Boglaienko, Dhruba J. Deka, Garam Lee, Trent R. Graham, Libor Kovarik, Yong Wang, János Szanyi, and Konstantin Khivantsev **Mechanistic insights into adsorptive and catalytic reactions from controllable distributions of metal cations (Pd, Pt. Ni, Cr, Cu) as $[M–OH]^{+1}$/1Al or M^{2+}/2Al in zeolites** *Angewandte Chemie International Edition* 2025 64, e202516086 DOI: 10.1002/anie.202516086

3. Dinh Nhat Dang Nguyen, Bar Mosevitzky Lis, Mingyu Guo, Wenda Hu, Nicholas R. Jaegers, Qingling Liu, Caixia Liu, Yong Wang, Jian Zhi Hu, and Israel E. Wachs **Effect of promoters (CeOx, ZrOx, and SiOx) on activity and selectivity in the presence of H_2O for selective catalytic reduction (SCR) of NO with NH_3 by supported V_2O_5/TiO_2 catalysts** *Applied Catalysis B* 2026 382, 125942 DOI: 10.1016/j.apcatb.2025.125942

4. Nicholas R. Jaegers, Mikalai Artsiusheuski, Vardan Danghyan, Junnan Shangguan, Carlos Lizandara Pueyo, and Enrique Iglesia **Hydrogenation of alkenes, cycloalkenes, and arene side chains at Lewis acid-base pairs: Kinetics, elementary steps, and thermodynamic implications for reverse reactions** *ACS Catalysis* 2025 15, 12610 DOI: 10.1021/acscatal.5c03523

2024

5. Nicholas R. Jaegers, Vardan Danghyan, Junnan Shangguan, Carlos Lizandara Pueyo, Prashant Deshlahra, and Enrique Iglesia **Heterolytic C–H activation routes in catalytic dehydrogenation of light alkanes on Lewis acid-base pairs at ZrO_2 surfaces** *Journal of the American Chemical Society* 2024 146, 25710 DOI: 10.1021/jacs.4c07766

6. Dongmin Yun, Nicholas R. Jaegers, Jian Zhi Hu, José E. Herrera, and Yong Wang; **Surface anchoring requirements for vanadia clusters on titanium oxide surfaces and their impact on activity for oxidative dehydrogenation of ethanol** *Journal of Catalysis* 2024 437, 115642 DOI: 10.1016/j.jcat.2024.115642

7. Ji Yang, Chaochao Dun, Lorenz J. Falling, Qi Zheng, Jeng-Lung Chen, Miao Zhang, Nicholas R. Jaegers, Chirthra Asokan, Jinghua Guo, Miquel Salmeron, David Prendergast, Yanbing Guo, Jeffrey J. Urban, Gabor A. Somorjai, Yanbing Guo, and Ji Su **Unveiling highly sensitive active site in atomically dispersed gold catalysts for enhanced ethanol dehydrogenation** Angewandte Chemie International Edition 2024 63, e202408894 DOI: 10.1002/anie.202408894

2023

8. Konstantin Khivantsev, Miroslaw A. Derewinski, Libor Kovarik, Mark Bowden, Nicholas R. Jaegers, Daria Boglaienko, Xavier Isidro Pereira Hernandez, Carolyn Pearce, Yong Wang, and János Szanyi **Increasing Al-pair abundance in SSZ-13 zeolite via zeolite synthesis in the presence of alkaline earth metal hydroxide produces hydrothermally stable Co-, Cu- and Pd-SSZ-13 materials** *Catalysts* 2024 14, 56 DOI: 10.3390/catal14010056

9. Sungmin Kim, Nicholas R. Jaegers, Wenda Hu, Jian Zhi Hu, Feng Chen, Qiang Liu, Donald Camaioni, Miroslaw Derewinski, Oliver Gutiérrez, Yue Liu, and Johannes Lercher **Impact of the environment of BEA-type zeolites for sorption of water and cyclohexanol** *The Journal of Physical Chemistry C* 2023 127, 23390-23399 DOI: 10.1021/acs.jpcc.3c05405

10. Nicholas R. Jaegers and Enrique Iglesia **Theoretical assessment of the mechanism and active sites for alkene dimerization on Ni monomers grafted onto mesoporous aluminosilicates: $(Ni\text{-}OH)^+$ centers and C-C coupling mediated by Lewis acid-base pairs** *Journal of the American Chemical Society* 2023 145, 6349–6361 DOI: 10.1021/jacs.2c13487

11. Konstantin Khivantsev, Nicholas R. Jaegers, Hristiyan Aleksandrov, Inhak Song, Xavier Pereira-Hernandez, Mark Engelhard, Jinshu Tian, Linxiao Chen, Debora Motta Meira, Libor Kovarik, Georgi Vayssilov, Yong Wang, and János Szanyi **Single Ru(II) ions on ceria as highly active catalyst for abatement of NO** *Journal of the American Chemical Society* 2023 145, 5029–5040 DOI: 10.1021/jacs.2c09873

12. Nicholas R. Jaegers, Nancy M. Washton, Yong Wang, and Jian Zhi Hu; **High-field NMR spectroscopy** In: I. Wachs, M. Bañares (eds) *Springer Handbook of Advanced Catalyst Characterization*, Springer, Cham 2023 DOI: 10.1007/978-3-031-07125-6_34

2022

13. Fan Lin, Wenda Hu, Nicholas R. Jaegers, Feng Gao, Jian Zhi Hu, Huamin Wang, and Yong Wang **Elucidation of the roles of water on the reactivity of surface intermediates in carboxylic acid ketonization on TiO_2** *Journal of the American Chemical Society* 2022 145, 99–109 DOI: 10.1021/jacs.2c08511

14. Trent R. Graham, Jian Zhi Hu, Nicholas R. Jaegers, Xin Zhang, Carolyn I. Pearce, and Kevin M. Rosso **NMR and Raman spectroscopy identifies an amorphous sodium aluminate hydrate phase mediating aluminum coordination change in highly alkaline sodium hydroxide solutions** *Inorganic Chemistry Frontiers* 2022 9, 6344–6357 DOI: 10.1039/d2qi01642g

15. Konstantin Khivantsev, Ja-Hun Kwak, Nicholas R. Jaegers,* Miroslaw A. Derewinski, and János Szanyi **Identification of the mechanism of NO reduction with ammonia (SCR) on zeolite catalysts** *Chemical Science* 2022 13, 10383–10394 DOI: 10.1039/d2sc00350c

16. Wenda Hu, Nicholas R. Jaegers, Austin Winkelman, Shiva S. Murali, Karl T. Mueller, Yong Wang, and Jian Zhi Hu **Modelling complex molecular interactions in catalytic materials for energy storage and conversion in nuclear magnetic resonance** *Frontiers in Catalysis* 2022 2 935174 DOI: 10.3389/fctls.2022.935174 [Topical]

17. Konstantin Khivantsev, Nicholas R. Jaegers,* Libor Kovarik, Ja-Hun Kwak, Miroslaw Derewinski, and János Szanyi **On the nature of extra-framework aluminum species in steamed zeolites** *Molecules* 2022 27, 2352 DOI: 10.3390/molecules27072352

18. Jian Zhi Hu, Nicholas R. Jaegers, Nathan T. Hahn, Wenda Hu, Kee Sung Han, Ying Chen, Jesse A. Sears, Viajay Murugesan, Kevin R. Zavadil, and Karl T. Mueller **Understanding the solvation-dependent properties of cyclic ether multivalent electrolytes using High Field NMR and Quantum Chemistry** *JACS Au* 2022 2, 917–932 DOI: 10.1021/jacsau.2c00046 [Supplementary Cover]

2021

19. Konstantin Khivantsev, Xinyi Wei, Libor Kovarik, Nicholas R. Jaegers, Eric D. Walter, Pascaline Tran, Yong Wang, and János Szanyi **Palladium/Ferrierite vs Palladium/SSZ-13 Passive NOx Adsorbers: Adsorbate-controlled Location of Atomically Dispersed Palladium (II) in Ferrierite Determines High Activity and Stability** *Angewandte Chemie International Edition* 2022 61, e202107554 DOI: 10.1002/anie.202107554

20. Konstantin Khivantsev, Nicholas R. Jaegers, Hristiyan A. Aleksandrov, Libor Kovarik, Miroslaw A. Derewinski, Yong Wang, Georgi N. Vayssilov, and János Szanyi **Biomimetic CO oxidation below -100 °C by a nitrate-containing metal-free microporous system** *Nature Communications* 2021 12, 6033 DOI: 10.1038/s41467-021-26157-3

21. Jun-Kun Lai, Nicholas R. Jaegers, Bar Mosevitzky Lis, Mingyu Guo, Michael E. Ford, Eric Walter, Yong Wang, Jian Zhi Hu, and Israel E. Wachs; **Structure-Activity Relationships of Hydrothermally Aged Titania-Supported Vanadium-Tungsten Oxide Catalysts for SCR of NO_X with NH_3** *ACS Catalysis* 2021 11, 12096–12111 DOI: 10.1021/acscatal.1c02130

22. Nicholas R. Jaegers, Yong Wang, Jian Zhi Hu, and Israel Wachs **Impact of Hydration on Supported V_2O_5/TiO_2 Catalysts as Explored by Magnetic Resonance Spectroscopy** *The Journal of Physical Chemistry C* 2021 125, 16766–16775 DOI: 10.1021/acs.jpcc.1c04150

23. Houqian Li, Dezhou Guo, Nisa Ulumuddin, Nicholas R. Jaegers, Junming Sun, Bo Peng, Jean-Sabin McEwen, Jian Zhi Hu, and Yong Wang **Elucidating the cooperative roles of water and Lewis acid-base pairs in cascade C-C coupling and self-deoxygenation reactions** *JACS Au* 2021 1, 1471–1487 DOI: 10.1021/jacsau.1c00218

24. Konstantin Khivantsev, Nicholas R. Jaegers, Ja-Hun Kwak, János Szanyi, and Libor Kovarik; **Precise identification of catalytically active sites on the surface of γ-alumina** *Angewandte Chemie International Edition* 2021 133, 17663–17671 DOI: 10.1002/anie.202102106

25. Kee Sung Han, Nathan T. Hahn, Nicholas R. Jaegers, Ying Chen, Jian Zhi Hu, Kevin R. Zavadil, M. Vijayakumar, and Karl T. Mueller **Factors Influencing Preferential Anion Interactions during Solvation of Multivalent Cations in Ethereal Solvents** *The Journal of Physical Chemistry C* 2021 125, 6005–6012 DOI: 10.1021/acs.jpcc.0c09830

26. Nicholas R. Jaegers, Thomas J. Weber, and Jian Zhi Hu **Low-temperature (< 200 °C) degradation of electronic nicotine delivery system liquids generates toxic aldehydes** *Scientific Reports* 2021 11, 7800 DOI: 10.1038/s41598-021-87044-x [Top 100 of 2021]

27. Suochang Xu, Nicholas R. Jaegers, Wenda Hu, Ja Hun Kwak, Xinhe Bao, Junming Sun, Yong Wang, and Jian Zhi Hu **High Field One-Dimensional and Two-Dimensional ^{27}Al Magic-Angle Spinning Nuclear Magnetic Resonance Study of θ-, δ-, or γ-Al_2O_3 Dominated Aluminum Oxides: Toward Understanding the Al Sites in γ-Al_2O_3** *ACS Omega* 2021 6, 4090–4099 DOI: 10.1021/acsomega.0c06163 [Supplementary Cover]

28. Konstantin Khivantsev, Nicholas R. Jaegers, Libor Kovarik, Meng Wang, Jian Zhi Hu, Yong Wang, Miroslaw A. Derewinski, and János Szanyi; **The Superior Hydrothermal Stability of Pd/SSZ-39 in Low Temperature Passive NOx Adsorption (PNA) and Methane Combustion** *Applied Catalysis B* 2021 280 119449 DOI: 10.1016/j.apcatb.2020.119449

2020

29. Fan Lin, Huamin Wang, Yuntao Zhao, Jia Fu, Donghai Mei, Nicholas R. Jaegers, Feng Gao, and Yong Wang **Elucidation of Active Sites in Aldol Condensation of Acetone over Single-Facet Dominant Anatase TiO_2 (101) and (001) Catalysts** *JACS Au* 2021 1, 41–52 DOI: 10.1021/jacsau.0c00028

30. Manish Shetty, Huamin Wang, Feng Chen, Nicholas R. Jaegers, Yue Liu, Donald M. Camaioni, Oliver Y. Gutierrez, and Johannes A. Lercher; **Directing the rate-enhancement for hydronium ion catalyzed dehydration via organization of alkanols in nanoscopic confinements** *Angewandte Chemie International Edition* 2021 60, 2304–2311 DOI: 10.1002/anie.202009835

31. Nicholas R. Jaegers, Wenda Hu, Yong Wang, Jian Zhi Hu **High Temperature and High Pressure In Situ Magic Angle Spinning Nuclear Magnetic Resonance Spectroscopy** *Journal of Visualized Experiments* 2020 DOI: 10.3791/61794

32. Konstantin Khivantsev, Carlos Vargas, Jinshu Tian, Libor Kovarik, Nicholas R. Jaegers, János Szanyi, and Yong Wang; **Economizing on Precious Metals in Three-Way Catalysts: Thermally Stable and Highly Active Single-Atom Rhodium on Ceria for NO Abatement under Dry and Industrially Relevant Conditions** *Angewandte Chemie International Edition* 2021 60, 391–398 DOI: 10.1002/anie.202010815

33. Ying Chen, Nicholas R. Jaegers, Hui Wang, Kee Sung Han, Jian Zhi Hu, Karl T. Mueller, and Vijayakumar Murugesan **Role of Solvent Rearrangement on Mg^{2+} Solvation Structures in Dimethoxyethane Solutions Using Multimodal NMR Analysis** *The Journal of Physical Chemistry Letters* 2020 11,6443–6449 DOI: 10.1021/acs.jpclett.0c01447

34. Libor Kovarik, Mark Bowden, Amity Anderson, Nicholas R. Jaegers, Nancy Washton, Dachuan Shi, János Szanyi, and Chuck Peden **Quantification of High Temperature Transition Al_2O_3 and Their Phase Transformations** *Angewandte Chemie International Edition* 2020 132, 21903–21911 DOI: 10.1002/anie.202009520

35. Vanessa Lebarbier Dagle, Austin Winkelman, Nicholas R. Jaegers, Johnny Saavedra-Lopez, Jian Zhi Hu, Mark H. Engelhard, Susan E. Habas, Sneha Akhade, Vassilliki-Alexandra Glezakou, Roger Rousseau, Yong Wang, and Robert A. Dagle; **Single-step conversion of ethanol to n-butenes over Ag-ZrO_2/SiO_2 catalysts** *ACS Catalysis* 2020 10, 10602–10613 DOI: 10.1021/acscatal.0c02235 [Back Cover]

36. Houqian Li, Jifeng Pang, Nicholas R. Jaegers, Libor Kovarik, Mark Engelhard, Anthony W. Savoy, Jian Zhi Hu, Junming Sun, and Yong Wang; **Conversion of ethanol to 1,3-butadiene over AgZrO2 based catalysts: the role of surface interfaces** *Journal of Energy Chemistry* 2021 54, 7–15 DOI: 10.1016/j.jechem.2020.05.038

37. Trent R. Graham, Mateusz Dembowski, Jian Zhi Hu, Nicholas R. Jaegers, Xin Zhang, Sue B. Clark, Carolyn I. Pearce, and Kevin M. Rosso; **Intermediate Species in the Crystallization of Sodium Aluminate Hydroxy Hydrates** *The Journal of Physical Chemistry C* 2020 124, 12337–12345 DOI: 10.1021/acs.jpcc.0c00205 [Supplementary Cover]

38. Ying Chen, Nicholas R. Jaegers, Kee Sung Han, Hui Wang, Robert P. Young, Garvit Agarwal, Andrew Lipton, Rajeev S. Assary, Nancy M. Washton, Jian Zhi Hu, Karl T. Mueller, and Vijayakumar Murugesan; **Probing Conformational Evolution and Associated Dynamics of $Mg(N(SO_2CF_3)_2)_2$·Di-methoxyethane Adduct Using Solid-state ^{19}F and ^{1}H NMR** *The Journal of Physical Chemistry C* 2020 124 (9), 4999–5008 DOI: 10.1021/acs.jpcc.9b10212

39. Nicholas R. Jaegers, Yong Wang, and Jian Zhi Hu; **Thermal perturbation of NMR properties in small polar and non-polar molecules** *Scientific Reports* 2020 10 (1), 6097 DOI: 10.1038/s41598-020-63174-6

40. Nicholas R. Jaegers, Karl T. Mueller, Yong Wang, and Jian Zhi Hu; **Variable Temperature, Pressure Operando MAS NMR for Catalysis Science and Related Materials** *Accounts of Chemical Research* 2020 53, 611–619 DOI: 10.1021/acs.accounts.9b00557 [Supplementary Cover]

41. Konstantin Khivantsev, Nicholas R. Jaegers, Iskra Z. Koleva, Hristiyan A. Aleksandrov, Libor Kovarik, Mark H. Engelhard, Feng Gao, Yong Wang, Georgi N. Vayssilov, and János Szanyi; **Stabilization of Super Electrophilic Pd^{+2} Cations in Small-Pore SSZ-13 Zeolite** *The Journal of Physical Chemistry C* 2020 124, 1, 309–321 DOI: 10.1021/acs.jpcc.9b06760

2019

42. Nicholas R. Jaegers; **Applications of In Situ Magnetic Resonance Spectroscopy for Structural Analysis of Oxide-Supported Catalysts** 2019 Washington State University, PhD dissertation, ProQuest: 27544902

43. Nicholas R. Jaegers,* Konstantin Khivantsev, Libor Kovarik, Daniel W. Klas, Jian Zhi Hu, Yong Wang, and János Szanyi; **Catalytic Activation of Ethylene C-H Bonds on Uniform D^8 Ir(I) and Ni(II) Cations in Zeolites: Towards Molecular level Understanding of Ethylene Polymerization on Heterogeneous Catalysts** *Catalysis Science & Technology* 2019 9, 6570–6576 DOI: 10.1039/C9CY01442J [2019 HOT Article, Inside Back Cover]

44. Trent R. Graham, Jianzhi Hu, Xin Zhang, Mateusz Dembowski, Nicholas R. Jaegers, Chuan Wan, Andrew R. Felmy, Sue B. Clark, Kevin M. Rosso, and Carolyn I. Pearce; **Unraveling Gibbsite Transformation Pathways in Concentrated Lithium Hydroxide** Inorganic *Chemistry* 2019 58, 12385–12394 DOI: 10.1021/acs.inorgchem.9b02000 [Supplementary Cover]

45. Jian Zhi Hu, Nicholas R. Jaegers, Ying Chen, Kee Sung Han, Hui Wang, Vijayakumar Murugesan, and Karl T. Mueller; **Adsorption and thermal decomposition of electrolytes on nanometer magnesium oxide: An in situ ^{13}C MAS NMR Study** *ACS Applied Materials & Interfaces* 2019 11, 38689–38696 DOI: 10.1021/acsami.9b11888 [Supplementary Cover]

46. Konstantin Khivantsev, Nicholas R. Jaegers, Libor Kovarik, Jian Zhi Hu, Yong Wang, Feng Gao, and János Szanyi; **Palladium/Zeolite Low Temperature Passive NO_X Adsorbers (PNA): Structure-adsorption property relationships for hydrothermally aged PNA materials** *Emission Control Science and Technology* 2020 6:126–138 DOI: 10.1007/s40825-019-00139-w

47. Xin Zhang, Wenwen Cui, Jian Zhi Hu, Hsiu-Wen Wang, Micah Prange, Chuan Wan, Nicholas R. Jaegers, Meirong Zong, Carolyn Pearce, Ping Li, Zheming Wang, Sue B. Clark, Kevin M. Rosso; **Transformation of Gibbsite to Boehmite in Caustic Aqueous Solution at Hydrothermal Conditions** *Crystal Growth and Design* 2019 19, 5557–5567 DOI: 10.1021/acs.cgd.9b00468

48. Nicholas R. Jaegers, Jun-Kun Lai, Yang He, Eric Walter, David A. Dixon, Ying Chen, Chongmin Wang, Mary Y. Hu, Karl T. Mueller, Israel E. Wachs, Yong Wang, and Jian Zhi Hu; **Mechanism by which Tungsten Oxide Promotes the Activity of Supported V_2O_5/TiO_2 Catalysts for NOx Abatement: Structural Effects Revealed**

by ^{51}V MAS NMR Spectroscopy *Angewandte Chemie International Edition* 2019 131, 12739–12746 DOI: 10.1002/anie.201904503 [Inside Back Cover]

49. Meng Wang, Nicholas R. Jaegers, Mal Soon Lee, Chuan Wan, Jian Zhi Hu, Hui Shi, Donghai Mei, Sarah D. Burton, Donald M. Camaioni, Oliver Y. Gutierrez, Vassiliki-Alexandra Glezakou, Roger Rousseau, Tong Wang, and Johannes A. Lercher; **Genesis and Stability of Hydronium Ions in Zeolite Channels** *Journal of the American Chemical Society* 2019 141 (8), 344–3455 DOI: 10.1021/jacs.8b07969

50. Konstantin Khivantsev, Nicholas R. Jaegers, Libor Kovarik, Sebastian Prodinger, Miroslaw A Derewinski, Yong Wang, Feng Gao, and János Szanyi; **Palladium/Beta Zeolite Passive NOx Adsorbers (PNA): Clarification of PNA Chemistry and the Effects of CO and Zeolite Crystallite Size on PNA Performance** *Applied Catalysis: A, General* 2019 569, 141–148 DOI: 10.1016/j.apcata.2018.10.021 [CHF Peden Special Issue]

2018

51. Xin Zhang, Patricia I. Huestis, Carolyn I. Pearce, Jian Zhi Hu, Katherine Page, Lawrence M. Anovitz, Alexander Aleksandrov, Micah P. Prange, Sebastien N. Kerisit, Mark E. Bowden, Wenwen Cui, Zheming Wang, Nicholas R. Jaegers, Trenton R. Graham, Mateusz Dembowski, Hsiu-Wen Wang, Jue Liu, Alpha T N'Diaye, Markus Bleuel, David Mildner, Thomas Michael Orlando, Gragory A. Kimmel, Jay Laverne, Sue B. Clark, and Kevin M. Rosso; **Boehmite and Gibbsite Nanoplates for the Synthesis of Advanced Alumina Products** *ACS Applied Nano Materials* 2018 1 (12), 7115–7128 DOI: 10.1021/acsanm.8b01969

52. Konstantin Khivantsev, Nicholas R. Jaegers, Libor Kovarik, Jonathan Hanson, Xiaoyan Zhang, Franklin Tao, Iskra Z. Koleva, Hristiyan A. Aleksandrov, Georgi Vayssilov, Yong Wang, Feng Gao, and János Szanyi; **Achieving Atomic Dispersion of Highly Loaded Transition Metals in Small-pore Zeolite SSZ-13: a New Class of High-capacity and High-efficiency Low Temperature Passive NOx and CO Adsorbers** *Angewandte Chemie International Edition* 2018 130, 16914–16919 DOI: 10.1002/ange.201809343 [Back cover]

53. Jian Zhi Hu, Nicholas R. Jaegers, Mary Y. Hu, and Karl T. Mueller; **In Situ and Ex Situ NMR for Battery Research** *Journal of Physics: Condensed Matter* 2018 30 463001 DOI: 10.1088/1361-648X/aae5b8

54. Trenton R. Graham, Mateusz Dembowski, Baez E. Martinez, Xin Zhang, Nicholas R. Jaegers, Jian Zhi Hu, Hsiu-Wen Wang, Miroslaw S. Gruszkiewicz, Andrew G. Stack, Mark E. Bowden, Calvin H. Delegard, Gregor K. Schenter, Aurora E. Clark, Sue B. Clark, Andrew R. Felmy, Kevin M. Rosso, and Carolyn I. Pearce; **In-Situ ^{27}Al NMR Spectroscopy of Aluminate in Sodium Hydroxide Solutions Above and Below Saturation with Respect to Gibbsite** *Inorganic Chemistry* 2018 57, 11864–11873 DOI: 10.1021/acs.inorgchem.8b00617

55. Jian Zhi Hu, Nav Nidhi Rajput, Chuan Wan, Yuyan Shao, Xuchu Deng, Nicholas R. Jaegers, Mary Hu, Yingwen Chen, Yongwoo Shin, Joshua Monk, Zhong Chen, Zhaohai Qin, Karl Todd Mueller, Jun Liu, and Kristin Persson; **^{25}Mg NMR and Computational Modeling Studies of the Solvation Structures and Molecular Dynamics in Magnesium Based Liquid Electrolytes** *Nano Energy* 2018 46 436–446 DOI: 10.1016/j.nanoen.2018.01.051

2017

56. Nicholas R. Jaegers, Mary Y. Hu, David W. Hoyt, Yong Wang, and Jian Zhi Hu; **Development and application of in-situ high-temperature, high-pressure magic angle spinning NMR** In: G. Webb *Modern Magnetic Resonance, 2nd edition,* Springer, Cham DOI: 10.1007/978-3-319-28388-3_93

57. Jian Zhi Hu, Xin Zhang, Nicholas R. Jaegers, Chuan Wan, Mary Y. Hu, Trenton R. Graham, Carolyn I. Pearce, Andrew R. Felmy, Sue B. Clark, and Kevin M. Rosso; **Transitions in Al Coordination during Gibbsite Crystallization using High-Field ^{27}Al and ^{23}Na MAS NMR Spectroscopy** *The Journal of Physical Chemistry C* 2017 121 (49), 27555–27562 DOI: 10.1021/acs.jpcc.7b10424

58. Nicholas R. Jaegers, Chuan Wan, Mary Y. Hu, Monica Vasiliu, David A. Dixon, Eric Walter, Israel E. Wachs, Yong Wang, and Jian Zhi Hu, **Investigation of Silica-Supported Vanadium Oxide Catalysts by High-Field ^{51}V Magic-Angle Spinning NMR** *The Journal of Physical Chemistry C* 2017 121 (11), 6246-6254 DOI: 10.1021/acs.jpcc.7b01658

2016

59. Chuan Wan, Mary Y. Hu, Nicholas R. Jaegers, Dachuan Shi, Huamin Wang, Feng Gao, Zhaohai Qin, Yong Wang, and Jian Zhi Hu; **Investigating the Surface Structure of γ-Al_2O_3 Supported WO_X Catalysts by High Field ^{27}Al MAS NMR and Electronic Structure Calculations** *The Journal of Physical Chemistry C* 2016 120 (40), 23093–23103 DOI: 10.1021/acs.jpcc.6b09060

PATENTS & APPLICATIONS

1. Mikalai Artsiusheuski, Nicholas R. Jaegers, Andrew Hwang, Enrique Iglesia, and Carlos Lizandara Pueyo **Process for preparing one or more arenes from one or more alkanes** [US Provisional Patent Application Filed]

2. Enrique Iglesia, Mikalai Artsiusheuski, Nicholas R. Jaegers, Carlos Lizandara Pueyo, Craig cain-Borgman, and Stephan A. Schunk **Metal oxide catalysts with exposed active Lewis acid-base pairs for catalytic valorization of long-chain alkanes and polyolefins** [US Provisional Patent Application Filed]

3. Enrique Iglesia, Mikalai Artsiusheuski, Nicholas R. Jaegers, Carlos Lizandara Pueyo, Roel Sigifredo Sanchez-Carrera, Craig Jon Cain-Borgman, Stephan A. Schunk, Sebastian Weber, Piyush Ingale, and Noah Subat, **Process for Preparing Metal and Mixed Metal Oxide Catalysts** [US Provisional Patent Application Filed]

4. Enrique Iglesia, Vardan Danghyan, Nicholas R. Jaegers, Junnan Shangguan, Carlos Lizandara Pueyo, Craig Jon Cain-Borman, Joseph Dellamorte, and Arunabha Kundu, **Lewis Acid Base Pairs as Highly Active Catalytic Sites for Hydrogenation and Dehydrogenation Processes** WO2024177986A2

5. Jian Zhi Hu, Nicholas R. Jaegers, Mary Hu, Wenda Hu, and Thomas Weber **An Electronic Cigarette Atomizer for a Reduction in Harmful Combustion By-Products** [US Provisional Patent Application Filed]

6. Konstantin Khivantsev, János Szanyi, Nicholas R. Jaegers, Libor Kovarik, Miroslaw A. Derewinski, and Yong Wang [US Provisional Patent Application Filed]

7. Konstantin Khivantsev, Libor Kovarik, János Szanyi, Yong Wang, Ja-Hun Kwak, and Nicholas R. Jaegers **Hydrothermally and thermally stable catalytic materials based on theta-alumina** US20220152585A1

8. Jian Zhi Hu, Nicholas R. Jaegers, Mary Y. Hu, and Mark Townsend **Magnetically coupled loading chamber and apparatus for in situ MAS NMR: Operating under either high or low pressure** US11486946B2

9. Konstantin Khivantsev, János Szanyi, Nicholas R. Jaegers, Libor Kovarik, Feng Gao, and Yong Wang **High-Capacity, Low-Temperature, Passive NOx and CO Adsorbers and Methods for Making Same** US11071966B2

MEETING AND INVITED PRESENTATIONS

1. Nicholas R. Jaegers* **Engineering active sites and supports for controlled hydrocarbon transformations** CISTAR Biannual Meeting, Chicago, IL September 5, 2025 (*Presenter – Oral) [Invited Talk]

2. Nicholas R. Jaegers* Janik Hence, Prashant Deshlahra, and Enrique Iglesia; **Heterolytic activation of H–H, O–H, and C–H bonds at Lewis acid-base pairs at oxide surfaces: site geometry, through-space interactions, and scaling relations** ACS National Meeting, Washington, D.C. August 17, 2025 (*Presenter – Oral) [Invited Talk]

3. Nicholas R. Jaegers*, Mikalai Artsiusheuski, Vardan Danghyan, Junnan Shangguan, Prashant Deshlahra, Carlos Lizandara Pueyo, and Enrique Iglesia; **Revealing the unique reactive properties of chemically-treated oxide surfaces for heterolytic C–H activation routes in catalysis** 29th North American Meeting (NAM) of the North American Catalysis Society, Atlanta, GA. June 13, 2025 (*Presenter – Oral)

4. Nicholas R. Jaegers* and Enrique Iglesia; **Heterolytic C–H activation routes in alkane dehydrogenation on Lewis acid-base pairs at ZrO_2 surfaces** Rocky Mountain Catalysis Society Symposium, Boulder, CO. April 21, 2025 (*Presenter – Oral) [Invited Talk]

5. Nicholas R. Jaegers*, Mikalai Artsiusheuski, Carlos Lizandara Pueyo, Roel Sanchez-Carrera, and Enrique Iglesia; **Experimental and computational nexus in heterolytic C–H activation on low-coordination Lewis acid-base pairs of anisotropic ZrO_2 catalysts** California Research Alliance Spring Review, Berkeley, CA. April 23, 2024 (*Presenter – Poster)

6. Nicholas R. Jaegers*, Vardan Danghyan, Junnan Shangguan, Biswanath Dutta, Carlos Lizandara-Pueyo, Janik Hence, Guang Miao, Joseph C. Dellamorete, Prashant Deshlahra, and Enrique Iglesia; **C–H activation of hydrocarbons on Lewis acid-base pairs of earth-abundant oxide nanostructures** ACS National Meeting, San Fransisco, CA. August 15, 2023. (*Presenter – Oral)

7. Nicholas R. Jaegers*, Vardan Danghyan, Junnan Shangguan, Biswanath Dutta, Carlos Lizandara-Pueyo, Janik Hence, Guang Miao, Joseph C. Dellamorete, Prashant Deshlahra, and Enrique Iglesia; **C–H activation of hydrocarbons on Lewis acid-base pairs of earth-abundant oxide nanostructures** ACS National Meeting, San Fransisco, CA. August 14, 2023. (*Presenter – Poster) [Sci Mix]

8. Nicholas R. Jaegers* and Jian Zhi Hu; **High-pressure, high-temperature MAS NMR for catalysis science** Global NMR Discussion Meetings Twitter Conference, July 19–21, 2023. (*Presenter – Video)

9. Nicholas R. Jaegers*, Vardan Danghyan, Junnan Shangguan, Janik Hence, Prashant Deshlahra, Carlos Lizandara Pueyo, and Enrique Iglesia; **Heterolytic C–H activation routes in catalytic dehydrogenation of C_2–C_7 alkanes on Lewis acid-base pairs on chemically-treated ZrO_2 surfaces** 28th North American Meeting (NAM) of the North American Catalysis Society, Providence, RI. June 18, 2023. (*Presenter – Oral)

10. Nicholas R. Jaegers*, Vardan Danghyan, Junnan Shangguan, Carlos Lizandara Pueyo, and Enrique Iglesia; **Non-oxidative dehydrogenation of alkanes on metal-oxide catalysts** California Research Alliance Spring Review, Berkeley, CA. April 19, 2023 (*Presenter – Poster)

11. Nicholas R. Jaegers*, Vardan Danghyan, and Enrique Iglesia; **Mechanistic assessment of dehydrogenation reactions of light alkanes: identity and kinetic relevance of elementary steps and inferences for hydrogenation reactions** California Research Alliance Fall Review, Santa Barbara, CA. November 3, 2022 (*Presenter – Oral)

12. Nicholas R. Jaegers*, Shuai Wang, Iker Agirrezabal-Telleria, and Enrique Iglesia; **Mechanistic assessments of alkene dimerization on cationic Ni species grafted within mesoporous solids** ACS National Meeting, Chicago, IL. August 21, 2022. (*Presenter – Poster) [Sci Mix]

13. Nicholas R. Jaegers*, Shuai Wang, Iker Agirrezabal-Telleria, and Enrique Iglesia; **Mechanistic assessments of alkene dimerization on cationic Ni species grafted within mesoporous solids** ACS National Meeting, Chicago, IL. August 21, 2022. (*Presenter – Oral, Symposium Presider)

14. Nicholas R. Jaegers*, Robert T. Carr, and Enrique Iglesia; **Assessment of structural and functional non-uniformity of dispersed VO_X and O_2 activation routes in Mars-van Krevelen Redox Cycles** 27th North American Meeting (NAM) of the North American Catalysis Society, New York, NY. May 25, 2022. (*Presenter – Oral)

15. Vardan Danghyan*, Nicholas R. Jaegers*, and Enrique Iglesia; **Non-oxidative dehydrogenation of alkanes on metal-oxide nanostructures** California Research Alliance Spring Review, Berkeley, CA. May 4, 2022 (*Presenter – Oral)

16. Vardan Danghyan*, Nicholas R. Jaegers*, Junnan Shangguan, Carlos Lizandara Pueyo, and Enrique Iglesia; **Non-oxidative dehydrogenation of alkanes on metal-oxide catalysts** California Research Alliance Fall Review, Online. November 16, 2021 (*Presenter – Poster)

17. Nicholas R. Jaegers*, Konstantin Khivantsev, Libor Kovarik, Jian Zhi Hu, Yong Wang, and János Szanyi; **Insights on Ethene Oligomerization with Supported d^8 Metal Atoms** UK Catalysis Conference 2021, Online. January 6, 2021 (*Presenter – Oral)

18. Nicholas R. Jaegers*, Konstantin Khivantsev, Libor Kovarik, Jian Zhi Hu, Yong Wang, and János Szanyi; **Mechanistic Understanding of Ethylene Polymerization with Isolated d^8 Metal Atoms in Zeolites** AIChE 2020 Annual Meeting, Online. November 18, 2020 (*Presenter – Oral)

19. Nicholas R. Jaegers*, Mary Hu, Meng Wang, Vanessa Dagle, Huamin Wang, Asanga Padmaperuma, Yong Wang, and Jian Zhi Hu; **Discerning the fundamental interactions of water with porous catalysts by in situ MAS NMR** ACS National Meeting, San Diego, CA. August 26, 2019 (*Presenter – Oral) [Invited Talk]

20. Nicholas R. Jaegers*, Mary Hu, Meng Wang, Vanessa Dagle, Huamin Wang, Asanga Padmaperuma, Yong Wang, and Jian Zhi Hu; **Discerning the fundamental interactions of water with porous catalysts by in situ MAS NMR** ACS National Meeting, San Diego, CA. August 26, 2019 (*Presenter – Poster) [Sci Mix]

21. Nicholas R. Jaegers*, Jun-Kun Lai, Yang He, Eric Walter, David Dixon, Monica Vasiliu, Ying Cheng, Chongmin Wang, Mary Hu, Karl Mueller, Israel Wachs, Yong Wang, and Jian Zhi Hu; **Resolving the promotional mechanism in supported vanadium oxide SCR catalysts** ACS National Meeting, San Diego, CA. August 28, 2019. (*Presenter – Oral)

22. Nicholas R. Jaegers*, Yong Wang, and Jian Zhi Hu; **Investigating Catalytic Function with Operando NMR** Pacific Coast Catalysis Society, Pullman, WA. August 9, 2019. (*Presenter – Poster)

23. Nicholas R. Jaegers*, Jun-Kun Lai, Yang He, Eric Walter, David Dixon, Ying Cheng, Israel Wachs, Yong Wang, and Jian Zhi Hu; **Vanadium-Based NOx Abatement: Clarity in Promotion** 26th North American Meeting (NAM) of the North American Catalysis Society, Chicago, IL. June 25, 2019. (*Presenter – Oral)

24. Nicholas R. Jaegers* **Modifying the Structural Properties of Titania-Supported Vanadium Oxide Catalysts** Gene and Lina Voiland School of Chemical Engineering and Bioengineering 2019 Seminar Series, Pullman, WA. January 28, 2019 (*Presenter – Oral) [Invited Talk]

25. Nicholas R. Jaegers*, Lu Zhang, Berlin Sudduth, Eric D. Walter, Mark H. Engelhard, Libor Kovarik, Mary Y. Hu, Feng Gao, Huamin Wang, Yong Wang, and Jian Zhi Hu; **Towards the Speciation and Reactivity of Facet-Controller Vanadium Oxide Catalysts** AIChE 2018 Annual Meeting, Pittsburgh, PA. November 1, 2018 (*Presenter – Oral)

26. Nicholas R. Jaegers*, Jun-Kun Lai, Israel Wachs, Jian Zhi Hu, and Yong Wang; **Structure-Function Insights for Supported Metal-Oxide Catalysis** PNNL Post Graduate Research Symposium, Richland, WA. August 21, 2018 (*Presenter – Poster)

27. Nicholas R. Jaegers*, Yang He, Chongmin Wang, Mary Y. Hu, Israel Wachs, Yong Wang, and Jian Zhi Hu; **Tungsten-incorporated vanadia SCR catalysts, a structural interpretation** 73rd American Chemical Society Northwest Regional Meeting (NORM), Richland, WA. June 25, 2018 (*Presenter – Oral)

28. Nicholas R. Jaegers*, Mary Y. Hu, Yong Wang, and Jian Zhi Hu; **High-pressure, thermally extensive MAS NMR for demystifying water** 73rd American Chemical Society Northwest Regional Meeting (NORM), Richland, WA. June 26, 2018 (*Presenter – Oral)

29. Nicholas R. Jaegers*, Chuan Wan, Mary Y. Hu, Monica Vasiliu, David A. Dixon, Eric D. Walter, Israel E. Wachs, Yong Wang, and Jian Zhi Hu; **Computationally-Enhanced Spectroscopic Studies of Supported Vanadium Oxide** 2017 AIChE Annual Meeting, Minneapolis, MN. November 1, 2017 (*Presenter – Oral)

30. Nicholas R. Jaegers*, Chuan Wan, Mary Y. Hu, Monica Vasiliu, David A. Dixon, Eric D. Walter, Israel E. Wachs, Yong Wang, and Jian Zhi Hu; **Spectroscopic and Theoretical Insights on Supported Vanadium Oxide** 25th North American Meeting (NAM) of the North American Catalysis Society, Denver, Co. June 6, 2017. (*Presenter – Poster)

MEDIA COVERAGE

- Karyn Hede, US Department of Energy "Faster and cheaper ethanol-to-jet-fuel on the horizon" *ScienceDaily* August 19, 2021. (https://www.sciencedaily.com/releases/2021/08/210819125236.htm)
- Lehigh University "Finally, the answer to a 'burning' 40-year-old question" *PHYS.ORG* October 24, 2019. (https://phys.org/news/2019-10-year-old.html)
- Rebekah Orton, PNNL "Identified: Molecular structure that breaks down important components of smog" *PHYS.ORG* August 22, 2019. (https://phys.org/news/2019-08-molecular-important-component-smog.html)
- Rebekah Orton, PNNL "Getting clear about clean air" PNNL Web Feature August 20, 2019. (https://www.pnnl.gov/news-media/getting-clear-about-clean-air)
- Institute for Integrated Catalysis "Getting real with catalysis research: PNNL spectroscopic capabilities mimic harsh conditions of industrial operations" *Transformations* July 24, 2019. (https://iic.pnnl.gov/news/transformations/harnessingNMR.stm)