

RACHITA RANA (*She/Her*)

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25 Ames St.
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CURRENT POSITION

Postdoctoral Associate MIT, Chemical Engineering Jan 2024 – Present
Advisor: Prof. Yuriy Romàn-Leshkov

EDUCATION

Ph.D. University California, Davis, Chemical Engineering. Oct 2019 – Dec 2023
Advisors: Prof. Ambarish R. Kulkarni, Prof. Simon R. Bare
GPA: 3.8/4.0

MS University of Saskatchewan, Chemical Engineering Jun 2014 – Dec 2017
Advisor: Prof. Ajay K. Dalai
GPA: 3.9/4.0

BS Banasthali University, Chemical Engineering Jul 2009 – May 2013

HONORS AND AWARDS

Kaufman Teaching Certificate Program (KTCP) 2024
AICHE WIC Travel Award 2024
NACS Travel Award for ICC Lyon 2024
MIT Rising Star (MIT ChemE) 2023
Best Poster at SUNCAT Summer Institute 2023
Kokes Award (NACS) 2023
Graduate Student Association Travel Award 2023
(University of California Davis)
Chemical Engineering Graduate Scholarship 2016
(University of Saskatchewan)
Graduate Student Travel Award 2016
(University of Saskatchewan)
Graduate Student Travel Award 2015
(University of Saskatchewan)
Five-fold Education All-Rounder Award 2013
(Banasthali University)

RESEARCH EXPERIENCE

Postdoc at MIT Feb 2024 – Present
Advisor: Yuriy Romàn-Leshkov

- Capacitive devices (catalytic condensers) fabrication (ALD, E-beam, clean room)
- Operando characterization using for thin film devices using atomic force microscopy, grazing angle spectroscopy (XAS, IR, XPS)
- Catalysis using promotional effect of electric field

Internship at SLAC and Stanford University July – Dec 2023

Advisors: Profs. Simon Bare & Matteo Cargnello

- Synthesis of tandem catalyst for epoxidation reaction
- Catalytic testing and *operando* XAS experiments

Computational Catalysis, UC Davis, USA 2019 – Present

Advisor: Prof. Ambarish R. Kulkarni

- Atomistic simulations for catalytic systems/Atomically dispersed catalyst
- Reaction barriers, phase diagrams and microkinetic modelling/ Atomically dispersed catalyst
- Development of QuantEXAFS– an automated workflow for EXAFS data analysis

XAS experiments, SSRL, USA 2021 – Present

Advisor: Profs. Simon Bare and Bruce Gates

- Ex-situ and operando experiments/Atomically dispersed catalyst
- Conventional and automated analysis of XAS data
- Synthesis and analyses of atomically dispersed catalysts

Experimental catalysis & XAS, USask & CLS, Canada 2018 – 2019

Advisor: Prof. Ajay Dalai and Dr. Yongfeng Hu

- Super-critical water gasification/Asphaltene and petcoke
- Ex-situ and operando experiments/spent catalyst

Experimental catalysis, York University, Canada 2017 – 2018

Advisor: Prof. Janusz Kozinski and Prof. Ajay Dalai

- Super-critical water gasification/hydrogen yields
- Continuous and batch reactions/various feedstock

Experimental catalysis, USask, Canada 2014 – 2017

Advisor: Prof. Ajay Dalai and Dr. John Adjaye

- Hydrotreating/Impact of process parameters catalyst deactivation
- Catalyst–fines chemical interaction/light gas oil, NiMo/ γ -Al₂O₃

Conducting thin films, DRDO, India 2012

Advisor: Dr. M. Nasim and Dr. Santosh K. Tripathi

- Fabricated polyimide (PI) films/thermal resistant films
- Spray pyrolysis, chemical vapor deposition, sol-gel and spin coater/synthesis and characterization of conducting indium tin oxide films

PUBLICATIONS & BOOK CHAPTERS (* CO-FIRST) (H-INDEX- 15; CITATIONS- 1110)

1. **Rana, R.**; Hong, J.; Hoffman, A. S.; Werghi, B.; Bare, S.; Kulkarni, A.; Quantifying the Site Heterogeneities of Non-uniform Catalysts using QuantEXAFS. *Chem. Methods*. **2024** (Accepted)
2. Levell, Z.; Le, J.; Yu, S.; Wang, R.; Ethirajan, S.; **Rana, R.**; Kulkarni, A.; Resasco, J.; Lu, D.; Cheng, J.; Liu, Y. Emerging Atomistic Modeling Methods for Heterogeneous Electrocatalysis. *Chem. Rev.* **2024**, *124* (14), 8620–8656. <https://doi.org/10.1021/acs.chemrev.3c00735>.
3. Shaw, W. J.; Kidder, M. K.; Bare, S. R.; Delferro, M.; Morris, J. R.; Toma, F. M.; Senanayake, S. D.; Autrey, T.; Biddinger, E. J.; Boettcher, S.; Bowden, M. E.; Britt, P. F.; Brown, R. C.; Bullock, R. M.; Chen, J. G.; Daniel, C.; Dorhout, P. K.; Efroymsen, R. A.; Gaffney, K. J.; Gagliardi, L.; Harper, A. S.; Heldebrant, D. J.; Luca, O. R.; Lyubovsky, M.; Male, J. L.; Miller, D. J.; Prozorov, T.; Rallo, R.; **Rana,**

- R.**; Rioux, R. M.; Sadow, A. D.; Schaidle, J. A.; Schulte, L. A.; Tarpeh, W. A.; Vlachos, D. G.; Vogt, B. D.; Weber, R. S.; Yang, J. Y.; Arenholz, E.; Helms, B. A.; Huang, W.; Jordahl, J. L.; Karakaya, C.; Kian, K.; Kothandaraman, J.; Lercher, J.; Liu, P.; Malhotra, D.; Mueller, K. T.; O'Brien, C. P.; Palomino, R. M.; Qi, L.; Rodriguez, J. A.; Rousseau, R.; Russell, J. C.; Sarazen, M. L.; Sholl, D. S.; Smith, E. A.; Stevens, M. B.; Surendranath, Y.; Tassone, C. J.; Tran, B.; Tumas, W.; Walton, K. S. A US Perspective on Closing the Carbon Cycle to Defossilize Difficult-to-Electrify Segments of Our Economy. *Nat. Rev. Chem.* **2024**, *8* (5), 376–400. <https://doi.org/10.1038/s41570-024-00587-1>.
- Chen, Y.*; **Rana, R.***; Zhang, Y.; Hoffman, A. S.; Huang, Z.; Yang, B.; Vila, F. D.; Perez-Aguilar, J. E.; Hong, J.; Li, X.; Zeng, J.; Chi, M.; Kronawitter, C. X.; Wang, H.; Bare, S. R.; Kulkarni, A. R.; Gates, B. C. Dynamic Structural Evolution of MgO-Supported Palladium Catalysts: From Metal to Metal Oxide Nanoparticles to Surface Then Subsurface Atomically Dispersed Cations. *Chem. Sci.* **2024**, *15*, 6454–6464. <https://doi.org/10.1039/d4sc00035h>.
 - Hiennadi, E. J.; Molajafari, F.; **Rana, R.**; Hoffman, A. S.; Bare, S. R.; Howe, J. D.; J. Khatib, S. Understanding the Control of Speciation of Molybdenum Oxides in MFI-Type Zeolites. *Chem. Mater.* **2023**, *35* (23), 9907–9923. <https://doi.org/10.1021/acs.chemmater.3c01545>.
 - Price, T.; **Rana, R.**; Ethirajan, S. K.; Holton, S. J.; Kulkarni, A. R. An Introductory Primer for Modeling Atomically Dispersed Catalysts Using Density Functional Theory. In *Comprehensive Computational Chemistry (CMPC)*; Jackson, L., Ed.; Elsevier, **2022**.
 - Rana, R.**; Vila, F. D.; Kulkarni, A. R.; Bare, S. R. Bridging the Gap between the X-Ray Absorption Spectroscopy and the Computational Catalysis Communities in Heterogeneous Catalysis: A Perspective on the Current and Future Research Directions. *ACS Catal.* **2022**, *12* (22), 13813–13830.
 - Felvey, N.; Guo, J.; **Rana, R.**; Xu, L.; Bare, S. R.; Gates, B. C.; Katz, A.; Kulkarni, A. R.; Runnebaum, R. C.; Kronawitter, C. X. Interconversion of Atomically Dispersed Platinum Cations and Platinum Clusters in Zeolite ZSM-5 and Formation of Platinum Gem-Dicarbonyls. *J. Am. Chem. Soc.* **2022**, *144* (30), 13874–13887. <https://doi.org/10.1021/jacs.2c05386>.
 - Chen, Y.*; **Rana, R.***; Huang, Z.; Vila, F. D.; Sours, T.; Perez-Aguilar, J. E.; Zhao, X.; Hong, J.; Ho, A. S.; Li, X.; Shang, C.; Blum, T.; Zeng, J.; Chi, M.; Salmeron, M.; Kronawitter, C. X.; Bare, S. R.; Kulkarni, A. R.; Gates, B. C. Atomically Dispersed Platinum in Surface and Subsurface Sites on MgO Have Contrasting Catalytic Properties for CO Oxidation. *J. Phys. Chem. Lett.* **2022**, *13*, 3896–3903. <https://doi.org/10.1021/acs.jpcclett.2c00667>.
 - Chen, Y.*; **Rana, R.***; Sours, T.*; Vila, F. D.; Cao, S.; Blum, T.; Hong, J.; Hoffman, A. S.; Fang, C. Y.; Huang, Z.; Shang, C.; Wang, C.; Zeng, J.; Chi, M.; Kronawitter, C. X.; Bare, S. R.; Gates, B. C.; Kulkarni, A. R. A Theory-Guided X-Ray Absorption Spectroscopy Approach for Identifying Active Sites in Atomically Dispersed Transition-Metal Catalysts. *J. Am. Chem. Soc.* **2021**, *143* (48), 20144–20156. <https://doi.org/10.1021/jacs.1c07116>.

11. **Rana, R.**; Nanda, S.; Reddy, S. N.; Dalai, A. K.; Kozinski, J. A.; Gökalp, I. Catalytic Gasification of Light and Heavy Gas Oils in Supercritical Water. *J. Energy Inst.* **2020**, *93* (5), 2025–2032. <https://doi.org/10.1016/j.joei.2020.04.018>.
12. Nanda, S.; **Rana, R.**; Vo, D. V. N.; Sarangi, P. K.; Nguyen, T. D.; Dalai, A. K.; Kozinski, J. A. A Spotlight on Butanol and Propanol as Next-Generation Synthetic Fuels. *Biorefinery Altern. Resour. Target. Green Fuels Platf. Chem.* **2020**, 1–494. <https://doi.org/10.1007/978-981-15-1804-1>.
13. Nanda, S.; **Rana, R.**; Hunter, H. N.; Fang, Z.; Dalai, A. K.; Kozinski, J. A. Hydrothermal Catalytic Processing of Waste Cooking Oil for Hydrogen-Rich Syngas Production. *Chem. Eng. Sci.* **2019**, *195*, 935–945. <https://doi.org/10.1016/j.ces.2018.10.039>.
14. **Rana, R.**; Nanda, S.; Maclennan, A.; Hu, Y.; Kozinski, J. A.; Dalai, A. K. Comparative Evaluation for Catalytic Gasification of Petroleum Coke and Asphaltene in Subcritical and Supercritical Water. *J. Energy Chem.* **2019**, *31*, 107–118. <https://doi.org/10.1016/j.jechem.2018.05.012>.
15. **Rana, R.**; Nanda, S.; Dalai, A. K.; Kozinski, J. A.; Adjaye, J. Synthetic Crude Processing. *In Fuel Processing and Energy Utilization*; **2019**; p 224. <https://doi.org/https://doi.org/10.1201/9780429489594>.
16. Okolie, J. A.; **Rana, R.**; Nanda, S.; Dalai, A. K.; Kozinski, J. A. Supercritical Water Gasification of Biomass: A State-of-the-Art Review of Process Parameters, Reaction Mechanisms and Catalysis. *Sustain. Energy Fuels* **2019**, *3* (3), 578–598. <https://doi.org/10.1039/c8se00565f>.
17. **Rana, R.**; Dalai, A. K.; Hu, Y.; Adjaye, J. Deposition of Fine Particles of Gas Oil on Hydrotreating Catalyst: Impact of Process Parameters and Filtration Trends. *Fuel Process. Technol.* **2018**, *171* (May 2017), 223–231. <https://doi.org/10.1016/j.fuproc.2017.09.019>.
18. Nanda, S.; **Rana, R.**; Sarangi, P. K.; Dalai, A. K.; Kozinski, J. A. A Broad Introduction to First-, Second-, and Third-Generation Biofuels. *In Recent Advancements in Biofuels and Bioenergy Utilization*; **2018**; pp 1–25. https://doi.org/10.1007/978-981-13-1307-3_1.
19. **Rana, R.**; Nanda, S.; Kozinski, J. A.; Dalai, A. K. Investigating the Applicability of Athabasca Bitumen as a Feedstock for Hydrogen Production through Catalytic Supercritical Water Gasification. *J. Environ. Chem. Eng.* **2018**, *6* (1), 182–189. <https://doi.org/10.1016/j.jece.2017.11.036>.
20. **Rana, R.**; Nanda, S.; Meda, V.; Dalai, A. K. A Review of Lignin Chemistry and Its Biorefining Conversion Technologies. *J. Biochem. Eng. Bioprocess Technol.* **2018**, *1* (2), 1–14.
21. Nanda, S.; **Rana, R.**; Zheng, Y.; Kozinski, J. A.; Dalai, A. K. Insights on Pathways for Hydrogen Generation from Ethanol. *Sustain. Energy Fuels* **2017**, *1* (6), 1232–1245. <https://doi.org/10.1039/C7SE00212B>.
22. **Rana, R.**; Badoga, S.; Dalai, A. K.; Adjaye, J. The Impact of Process Parameters on the Deposition of Fines Present in Bitumen-Derived Gas Oil on Hydrotreating Catalyst. *Energy and Fuels* **2017**, *31* (6), 5969–5981. <https://doi.org/10.1021/acs.energyfuels.7b00554>.
23. **Rana, R.**; Chakraborty, J.; Tripathi, S. K.; Nasim, M. Study of Conducting ITO Thin Film Deposition on Flexible Polyimide Substrate Using Spray Pyrolysis. *J.*

Nanostructure Chem. **2016**, 6 (1), 65–74. <https://doi.org/10.1007/s40097-015-0177-7>.

REVIEWER

Peer reviewed over **19 journal articles**- American Chemical Society journals (ACS Catalysis, JACS and Langmuir); Elsevier (Journal of Catalysis); Royal Society of Chemistry Journals, and nature communications. Reviewed abstracts for conferences – ICC and NAM

PRESENTATIONS

1. **Rana, R.**; Gates, B. C.; Kulkarni, A. R.; Bare, S. R. Probing the limits of “well-defined” atomically dispersed supported metal catalysts with experiment and theory. *18th ICC Lyon, France*; **2024**.
2. **Rana, R.**; Kulkarni, A. R.; Bare, S. R. Bridging the Gap between the Experimental and Computational Catalysis Communities: Recent Advances and Challenges. *AIChE Annual Meeting*; **2023**.
3. **Rana, R.**; Kulkarni, A. R.; Bare, S. R. Quantifying the Site Heterogeneity in Atomically Dispersed Catalyst Using Automated Workflow for XAS Analysis. *NAM 28 RI*; **2023**.
4. **Rana, R.**; Kulkarni, A. R.; Bare, S. R. QuantEXAFS: A Python-Based DFT Integrated Automated EXAFS Analysis Workflow. In *XAFS 2022 Sydney Australia*; **2022**.
5. **Rana, R.**; Chen, Y.; Huang, Z.; Zhao, X.; Hoffman, A. S.; Chi, M.; Vila, F. D.; Bare, S. R.; Gates, B. C. Atomically Dispersed Platinum on and in a MgO Support: Catalysts for CO Oxidation. In *NAM 27 NY*; **2021**.
6. **Rana, R.**; Chen, Y.; Gates, B. C.; Bare, S. R.; Kulkarni, A. R. QuantEXAFS : A Theory-Guided Approach for Quantitative Characterization of Atomically Dispersed Catalysts. In *NAM 27 NY*; **2021**.
7. **Rana, R.**; Dalai, A. K.; Adjaye, J. Deposition of Fines Entrained in Bitumen-Derived Light Gas Oil on Hydrotreating Catalyst: Impact of Process Parameters. In *NAM 25 Denver*; **2017**.
8. **Rana, R.**; Dalai, A. K.; Adjaye, J. Impact of Process Parameters on the Deposition of Fines Present in Bitumen-Derived Gas Oil in a Fixed-Bed Hydrotreater. In *ACS Meeting 2016*; **2016**.

TEACHING & MENTORING EXPERIENCE

University of California, Davis, USA

2020-2023

Teaching Assistant, Department of Chemical Engineering

- Taught, undergraduate courses averaging 120 students per semester, covering the following topics: **Lead TA– ECH 152B (Thermodynamics) twice, Lead TA– ECH 51 (Material Balance)**
- Graded exams and homework assignments
- Held bi-weekly office hours
- Coordinated grading with a team of 4

Mentoring at the University of California, Davis, USA

- 1 UG for python coding on a side project
- 2 first year Ph.D. in the lab for onboarding

- Regularly provided feedback on prelim and qualifying exam slides and presentations to various group members

University of Saskatchewan, Canada

2014 – 2016

Teaching Assistant, Department of Chemical Engineering

- Taught, undergraduate courses averaging 120 students per semester, covering the following topics: **ChE 464 (Petroleum production engineering)**, **ChE 423 (Process control and design)**, **ChE 223 (Thermodynamics)**, **GE 111 (General engineering laboratory instructor)**
- Developed quizzes, graded exams and homework assignments and held office hours
- Coordinated grading and labs with a team of 2-4 teaching assistants

Mentoring at the University of Saskatchewan, Canada

- 2 visiting scholars under **MITACS** program from India
- 1 from **Instituto Politécnico Nacional** (Mexico) during MS

PROFESSIONAL TRAINING (SEMINARS/WORKSHOPS)

- (1) **BNL XAFS short course, in-person** (Selected 2023)
- (2) **Modular Virtual Workshop on Future Needs for Interface Science Integrating Synchrotron Instrumentation, Theory, and Data** (Attended by Invite, 2022)
- (3) **IRASPA/RASPA workshop** (Certified, 2021)
- (4) **VISTA Symposium** (Certified, 2021)
- (5) **XAFS 2021 Conference**, Virtual, (Attended, 2021)
- (6) **Larch workshop**, Virtual, (Attended, 2021)
- (7) **OCEAN and CORVUS workshop**, SSRL User Meeting (Attended, 2021)
- (8) **FDMNES workshop** organized by Canadian Light Source, (Attended, 2020)
- (9) **BNL XAFS short course**, Virtual, (Selected, 2020)
- (10) **Theory, Application, and Tools for Multiscale Kinetic Modeling** (Attended, 2020)

OUTREACH/EXTRACURRICULAR ACTIVITIES

- (1) **AIChE Annual meeting 2024 Session Chair**
- (2) **ACS Catal Division Symposium Organizer for Fall 2024 meeting**
- (3) **ACS Fall 2024 Symposium Chair**
- (4) **AIChE Annual meeting 2023 Session Chair**
- (5) **SACNAS volunteer for K12 programs**
- (6) **K-12 science exhibition judge at AIChE**
- (7) **UG poster design mentor at UC Davis**
- (8) **Let's Talk Science Program Coordinator**
(University of Saskatchewan 2015-2016)
- (9) **Peer Mentor – Peer Assisted Learning Program**
(University of Saskatchewan 2015-2016)
- (10) **Executive Member – India Student Association**
(University of Saskatchewan 2014-2016)
- (11) **Radio Program Host at Community Radio, CFR 90.5 FM**
(City of Saskatoon, Saskatchewan 2014-2016)
- (12) **Member of the Editorial Board of the University Magazine– Ayam**
(Banasthali University, 2010-2013)