

# RACHITA RANA

□ Phone: (530) 505-1287  
✉ racrana@ucdavis.edu

1 Shields Ave  
Davis, CA 95616

## EDUCATION

<b>PhD</b>	<b>University California</b> , Davis, Chemical Engineering Advisors: Prof. Ambarish R. Kulkarni, Prof. Simon R. Bare GPA: 3.8/4.0	2019 – Present
<b>MS</b>	<b>University of Saskatchewan</b> , Chemical Engineering Advisor: Prof. Ajay K. Dalai GPA: 3.9/4.0	2014 – 2017
<b>BS</b>	<b>Banasthali University</b> , Chemical Engineering	2009 – 2013

## HONORS AND AWARDS

<b>Chemical Engineering Graduate Scholarship</b> University of Saskatchewan	2016
<b>Graduate Student Travel Award</b> University of Saskatchewan	2016
<b>Graduate Student Travel Award</b> University of Saskatchewan	2015
<b>Five-fold Education Award</b> Banasthali University	2013

## RESEARCH EXPERIENCE

<b>Computational Catalysis</b> , UC Davis, USA Advisor: Prof. Ambarish R. Kulkarni	2019 – Present
<b>XAS experiments</b> , SSRL, USA Advisor: Prof. Simon R. Bare	2021 – Present

• 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

• Ex-situ and operando experiments/Atomically dispersed catalyst  
• Conventional and automated analysis of XAS data

- Experimental catalysis & XAS**, USask & CLS, Canada 2018 – 2019  
Advisor: Prof. Ajay Dalai & 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, 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, Dr. John Adjaye
- Hydrotreating/Impact of process parameters catalyst deactivation
  - Catalyst–fines chemical interaction/light gas oil, NiMo/Al<sub>2</sub>O<sub>3</sub>
- Conducting thin films**, DRDO, India 2012  
Advisor: Dr. M. Nasim, 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

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## TEACHING EXPERIENCE

- 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
  - Held office hours
  - Coordinated grading and labs with a team of 2-4 teaching assistants
- University of California, Davis**, USA 2019 – Present  
**Teaching Assistant**, Department of Chemical Engineering
- Taught, undergraduate courses averaging 120 students per semester, covering the following topics: ECH 152B (Thermodynamics), ECH 51 (Material Balance)
  - Graded exams and homework assignments
  - Held office hours
  - Coordinated grading with a team of 4

## PUBLICATIONS

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- (1) **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**.
- (2) 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>.
- (3) **Rana, R.**; Chen, Y.; 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**.  
<https://doi.org/10.1021/acs.jpclett.2c00667>.
- (4) **Rana, R.**; Chen, Y.; 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>.
- (5) 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>.
- (6) **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>.
- (7) **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>.
- (8) 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>.
- (9) **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>.
- (10) 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>.
- (11) 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](https://doi.org/10.1007/978-981-13-1307-3_1).
- (12) **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>.
- (13) **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.
- (14) **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>.
- (15) **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>.
- (16) 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>.
- (17) **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>.

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## PRESENTATIONS

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- (1) **Rana, R.**; Kulkarni, A. R.; Bare, S. R. QuantEXAFS: A Python-Based DFT Integrated Automated EXAFS Analysis Workflow. In *XAFS 2022 Sydney Australia*; **2022**.
- (2) **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**.
- (3) **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**.
- (4) **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**.
- (5) **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**.
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## **PROFESSIONAL TRAINING**

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### **Seminar or Workshop**

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

## **OUTREACH/EXTRACURRICULAR ACTIVITIES**

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- (1) **Let's Talk Science Program Coordinator**  
(University of Saskatchewan 2015-2016)
- (2) **Peer Mentor – Peer Assisted Learning Program**  
(University of Saskatchewan 2015-2016)
- (3) **Executive Member – India Student Association**  
(University of Saskatchewan 2014-2016)
- (4) **Radio Program Host at Community Radio, CFR 90.5 FM**  
(City of Saskatoon, Saskatchewan 2014-2016)
- (5) **Member of the Editorial Board of the University Magazine– Aayam**  
(Banasthali University, 2010-2013)