Rajasi Shukre

Ph.D. Candidate Chemical Engineering Texas Tech University ⊠ rajasi.shukre@ttu.edu in rajasishukre

To understand and develop intensified process technologies for the manufacture of novel materials via experiments and computations.

Research Interests

- Molecular Simulations
- Metal Organic Frameworks
- o Biomass Pyrolysis

- Gas Adsorption
- o Continuous Crystallization
- Physical Characterization

Education

2016- Ph.D. (Chemical Engineering).

Present Maddox Engineering Research Centre, Texas Tech University

2010–2014 B.Tech (Chemical Engineering).

Laxminarayan Institute of Technology, India.

Professional Positions

2017 - Ph.D. Candidate, Texas Tech University,

Present Advisor: Dr. Chau-Chyun Chen,

Co-Advisors: Dr. Siva Vanapalli and Dr. Rajesh Khare

Thesis title: Synthesis of metal organic frameworks and understanding the thermodynamics of gas adsorption in such materials using molecular simulations

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June – Aug Summer Intern, RAPID Manufacturing Institute.

2021 • Molecular Simulations of Gas Adsorption Equilibria

o Modular Chemical Process Intensification

2014 – 2016 Process Engineer, Fluor Corp.

- Process Design of Fuel Gas Caustic Scrubber Unit in "Rotterdam Advanced Hydrocracker Project" of Exxon Mobil (Esso Nederland, B.V.)
- Development of Piping and Instrumentation Diagrams (P&ID).
- o HAZOP Study and Pressure Relief Valve Contingency Analysis.
- Co-ordination of multidisciplinary P&ID review meetings to notify Exxon Mobil of weekly updates.
- Review of vendor documents of Equipment.
- Hydraulic calculations of Control Valves in Sulfur Recovery Unit in "Clean Fuels Project" of Kuwait National Petroleum Company

June – Aug Summer Intern, Techint Corporation, India.

2013 o Heat Exchanger Design

• Pipeline insulation

Technical Skills

Computational

Languages: C, C++, MATLAB, Python, LATEX

Softwares: Aspen Properties, Aspen Plus, Aspen Hysys

Packages: RASPA, LAMMPS

Experimental

Material Characterization: SEM, BET, FTIR, PXRD Material Synthesis: Millifluidics, Batch Synthesis

o Other Tools

Visualization: VMD, OVITO Others: Fusion 360, 3D Printing

Teaching Experience

Spring 2019 **Transport Lab**, ChE 3232, Hosted Lab Sessions, graded performance of students during the sessions.

Fall 2018 Introduction to Chemical Processes and Engineering, ChE 2410, Graded assignments, hosted discussion sessions and office hours.

Publications

To access the updated list of my work, please visit my google scholar page.

- [1] Rajasi Shukre, Thomas Ericson, Daniel Unruh, Hannah Harbin, Sheima Khatib, Anthony Cozzolino, Siva Vanapalli and Chau-Chyun Chen. "Continuous Synthesis of HKUST-1 in a millifluidic reactor". In: (In preparation) (2021).
- [2] **Rajasi Shukre**, Rajesh Khare and Chau-Chyun Chen. "Estimation of binary interaction parameters of the aNRTL model using molecular simulations". In: (In preparation) (2021).
- [3] Gorensek, Maximilian B, **Shukre, Rajasi**, and Chen, Chau-Chyun. "Development of a thermophysical properties model for flowsheet simulation of biomass pyrolysis processes". In: *ACS Sustainable Chemistry & Engineering* 7.9 (2019), pp. 9017–9027.

Awards

- 2021 Graduate School Travel Fund Scholarship, Texas Tech University.
- 2020 Society of Plastics Engineers Scholarship, Texas Tech University Chapter.
- 2020-2021 Study Abroad Competitive Scholarship, Texas Tech University.
 - 2015 Recognition certificate for Front-End Engineering Deliverables, Exxon Mobil.

Contributed Conference Presentations

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- [1] Rajasi Shukre, Thomas Ericson, Daniel Unruh, Hannah Harbin, Sheima Khatib, Anthony Cozzolino, Siva Vanapalli and Chau-Chyun Chen. "Estimation of binary interaction parameters of the aNRTL model using molecular simulations (*Poster*)". In: *AICHE Fall Annual Meeting* (2021).
- [2] **Rajasi Shukre**, Rajesh Khare and Chau-Chyun Chen. "Estimation of binary interaction parameters of the aNRTL model using molecular simulations (*Poster*)". In: *AICHE Fall Annual Meeting* (2021).
- [3] Ban Caudle, **Rajasi Shukre** and Chau-Chyun Chen. "Modeling and Metrics Development for Biomass Pyrolysis Intensification Via Autothermal Operation". In: AICHE Spring Meeting and 15th Global Congress on Process Safety (2019).
- [4] Rajasi, Shukre and Chau-Chyun Chen. "Thermodynamic Modeling of CO₂ Absorption in Aqueous Amino Acid Salt Solutions with Symmetric Electrolyte NRTL Model". In: *AIChE Annual Meeting* (2018).

References

- Dr. Chau-Chyun Chen, chauchyun.chen@ttu.edu.
- Dr. Rajesh Khare, rajesh.khare@ttu.edu.
- Dr. Siva Vanapalli, siva.vanapalli@ttu.edu.