PUSHKAR GHANEKAR

Ph.D. Candidate at Purdue University

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SUMMARY

Chemical engineering Ph.D. candidate developing a molecular-level understanding of catalysts through a combination of chemistry, physics, and machine-learning (cheminformatics). My professional goal is to leverage my expertise in chemical sciences, data-wrangling, and AI model development, by being part of a cross-functional, data-driven team that develops solutions which enable accelerated design decisions.

EXPERIENCE

Graduate Research Assistant (Bill Murray Fellow)

Purdue University

Aug 2016 – Present West Lafayette, Indiana

- **Advisor:** Prof. Jeffrey P. Greeley
- 6 First-author Peer-reviewed Publications | 2 open-source Python packages | 1 Online-tool
- Computationally efficient tools to model complex catalysts:
  1. Graph neural networks to encode complex reaction surfaces
  2. Genetic algorithm to generate complex multi-component models hitherto deemed challenging (in collaboration with University of Florida)
- Catalyst active-site engineering & Investigating reaction mechanism:
  1. Collaborated with experimental group to propose design rules for building better catalysts for H2 production, propylene production, and exhaust emission control.
- Online lab-scale hazard evaluation and risk assessment platform:
  1. Developed an open-source tool to compile and scrutinize hazards-related information before performing experiments (in collaboration with CISTAR and Purdue Process Safety and Assurance Center)

Chemometrics & AI Intern

Dow Chemical Company

June 2020 – Aug 2020 Lake Jackson, Texas

- Developed ML model for small molecular screening. Scaled-up model inference capabilities resulting 30-fold improvement in compute time, increasing capability to screen potential molecules from millions to billions.
- Performed multivariate time-series analysis to troubleshoot complex manufacturing problems – proposed key variable driving the process deviation for plant-support team to detect anomaly, improving plant reliability & safety.

EDUCATION

Ph.D. in Chemical Engineering

Purdue University

2016 – Present West Lafayette, Indiana

Anticipated Graduation: Summer 2021

B.E. in Chemical Engineering

Institute of Chemical Technology

2012 – 2016 Mumbai, India

SKILLS

Mateiral informatics | Kinetic Modeling | Statistical Modeling | Multivariate Analysis | High-Performance Computing (GPU/CPU) | Linux/Bash | RDKit | Git | Python | PyData Stack | Graph Neural Networks | PyTorch | XGBoost | Dask | Web Scraping

RECENT COURSES

Deep Learning Specialization

deeplearning.ai

Feb 2020 Online

Data Science in ChE

Purdue University

Fall 2019 West Lafayette, Indiana

TEACHING

- Mentoring Graduate Student in the Research Group
- Design and Analysis of Processing Systems (ChE45000)
- Process Dynamics and Control (ChE45600)
- Graphic Designing using Adobe Photoshop (Mumbai, India)

OUTREACH

- Murdock Elementary School Teaching Volunteer
- Purdue Catalysis Center Webmaster
- CISTAR-SURF Highschool Teacher Mentor
- Purdue Cycling & Triathlon club member
- Citizens' Climate Lobby (Lafayette Chapter) volunteer