# PUSHKAR GHANEKAR, PH.D.

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# **SUMMARY**

Working on interesting ways to solve difficult problems. Passionate about leveraging data, science, and algorithms to fuel innovation and increase the quality of life.

### **EXPERIENCE**

Research Scientist (Cheminformatics)

### Eli Lilly Company

October 2021 - Present

Graduate Research Assistant (Bill Murray Fellow)

#### **Purdue University**

Marg 2016 - Aug 2021

♥ West Lafayette, Indiana

- Advisor: Prof. Jeffrey P. Greeley
- 8 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:
  - Tool to compile and scrutinize hazards-related information before performing experiments (in collaboration with CISTAR and Purdue Process Safety and Assurance Center)

#### Chemometrics & Al Intern

### **Dow Chemical Company**

🛗 June 2020 - Aug 2020

- **Q** Lake Jackson, Texas
- Developed a ML model for small molecular screening. Scaled-up model inference capabilities by 30-fold, increasing capability to screen potential molecules from millions to billions.
- Performed multivariate time-series analysis to detect operational anomalies and improving plant reliability & safety.

# **EDUCATION**

Ph.D. in Chemical Engineering

#### **Purdue University**

**#** 2016 - 2021

**♀** West Lafayette, Indiana

**Thesis:** Investigation of Multi-component Catalysts Functionality Using First-principles and Machine-learning

B.E. in Chemical Engineering

Institute of Chemical Technology

**2012 - 2016** 

Mumbai, India

## **SKILLS**

Cheminformatics

**Drug Discovery** 

Machine Learning

**Graph Neural Networks** 

Kinetic Modeling

Multivariate Analysis

Data Visualization

High-Performance Computing (GPU/CPU)

PyData Stack

Git

PyTorch

Web Scraping

# RECENT COURSES

Deep Learning Specialization deeplearning.ai

**♀** Online

Data Science in ChE

Purdue University

Fall 2019

**♀** West Lafayette, Indiana

# **TEACHING**

- Cheminformatics tool development mentoring
- Onboarding Graduate Students 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