

# PUSHKAR G. GHANEKAR, Ph. D. Candidate

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## PROFESSIONAL SUMMARY

Chemical engineering Ph.D. Candidate developing molecular-level understanding of catalysts through a combination of chemistry, physics, and machine-learning. My professional goal is to operate at the interface of industry/business functions, deriving intellectual and economic value. Orchestrate digitization of traditional research and manufacturing pipeline using domain expertise and AI/ML strategies fueling innovation.

## SKILLS AND TECHNOLOGIES

**Programming languages:** Python, Shell (Bash), HTML/CSS, JavaScript

**Technologies:** High-Performance Computing (CPU/GPU), PyTorch, XGBoost, Dask, RDKit, SIMCA, JMP, MATLAB, VASP/GPAW, Aspen plus, Adobe Photoshop, Blender

**Tools/packages:** Scikit-learn, Tableau/Plotly, NumPy, Pandas, Matplotlib, Selenium, BeautifulSoup, git, emacs

**Recent Coursework:** Deep learning specialization (deeplearning.ai), Data Science in ChE

## INDUSTRY EXPERIENCE

**Chemometric & AI Intern – Dow Chemical Company, Lake Jackson (Texas, USA)**

June - August 2020

**High throughput small-molecule screening (Core R&D):** Developed and deployed ML model for molecular discovery. Scaled-up model inference capabilities resulting 30-fold improvement in compute time, increasing capability to screen potential molecules from millions to billions. Benchmarked state-of-the-art chemistry-based deep-learning models for ligand design. Collaborated with Business R&D to validate model predictions.

**Anomaly detection & root-cause analysis:** Performed multivariate historical data analysis to troubleshoot complex manufacturing problems in collaboration with plant experts. Proposed key variables driving the manufacturing process upsets to detect anomaly at least 12 hours in advance, improving plant reliability & safety.

## RESEARCH EXPERIENCE

**Graduate Research Assistant (Bill Murray CISTAR Fellow)**

2016 – Ongoing

**Advisor:** Prof. Jeffrey Greeley

6 Peer-reviewed publications (2 accepted, 2 to be submitted, 2 in preparation) | 2 Open-source python packages | 1 Online-tool

### 1. Computationally efficient tools to model complex catalysts:

- First-ever extension of Graph Convolution Neural Networks to encode complex reaction surfaces. Accelerated screening of complex surface models to investigate complicated reaction dynamics made possible. Pioneered machine-learning application in the research group.
- Genetic algorithm to generate complex multi-component interfacial models hitherto deemed challenging, enhance understanding of chemical transformations (in collaboration with University of Florida)

### 2. Catalyst active-site engineering and investigating reaction mechanism:

- Collaborated with experimental group to propose design rules for building better catalysts through novel catalyst models and rigorous kinetic modeling for H<sub>2</sub> production and low-temperature Automotive Emission Control processes (in collaboration with research groups at Purdue, John Hopkins, Maryland, and Argonne National Lab)

### 3. Online lab-scale hazard evaluation and risk assessment platform:

- Open-source tool that provides a convenient platform to compile and scrutinize hazards-related information before performing experiments (in collaboration with CISTAR and Purdue Process Safety and Assurance Center)

## EDUCATION

**Ph.D. in Chemical Engineering (Anticipated graduation: June 2021)**

2016 – Ongoing

Purdue University (West Lafayette, Indiana) | GPA: 3.87/4.0

**B.E. in Chemical Engineering**

2012 – 2016

Institute of Chemical Technology (Mumbai, India) | GPA: 9.17/10.0 (First Class with Distinction)

## LEADERSHIP AND SERVICE

**Murdock Elementary Teaching Volunteer**

2017 - Present

Teaching introductory science and math concepts to third grader science club at local elementary school

**Purdue Catalysis Center Webmaster**

2018 - Present

Responsible for designing and maintaining Purdue Catalysis Center website <a href="#">[link]</a>	
<b>CISTAR-SURF Undergraduate Mentor</b>	May 2019
Taught fundamentals of high-performance computing, python, bash, and setup electronic structure calculations based on DFT	
<b>CISTAR-SURF Highschool Teacher Mentor</b>	May 2018
Advised a nation-wide cohort of high-school teachers on developing STEM courses focused on the basics of lab-scale reactions, high-performance computing, coding and basic algorithm development in the school curricula.	
<b>First-year Representative (Graduate Student Organization)</b>	2017 - 2018
Represent the incoming first-year graduate students. Organized mentor-mentee program and activities targeted to make the graduate school transition seamless for international students	
<b>Purdue Cycling and Triathlon club member</b>	2017 - Present
<b>Citizens' Climate Lobby (Lafayette Chapter) volunteer</b>	2019 - Present
<b>Technical Head and Core Organizing Team Member (Vortex 2014, Institute of Chemical Technology)</b>	2014 - 2015
Responsible for designing, building, and managing the festival website. Organized IDP (Industry Defined Problem) during Vortex 2014 (total participation 1500 students). Lead Designer involved in designing festival merchandise and apparels.	

## TEACHING AND MENTORING EXPERIENCE

• Mentoring 2 graduate students in the research group	Fall 2018 - Present
• Design and Analysis of Processing Systems (ChE45000)	Spring 2019
• Process Dynamics and Control (ChE45600)	Fall 2017
• Graphic Designing using Adobe Photoshop (Institute of Chemical Technology, India)	Spring 2016

## RESEARCH PUBLICATIONS

- **Ghanekar, P.**, Deshpande, S., et. al. , Versatile network motifs to encode geometric fingerprints and accelerate heterogeneous catalyst design, **in preparation**
- Talpade, A., **Ghanekar, P.** et. al. Promoting a safe laboratory environment using the Reactive Hazard Evaluation & Analysis Compilation Tool (RHEACT), **in preparation**
- V.S. Chaitanya Kolluru, **Ghanekar, P.**, et. al., Grand Canonical Evolutionary Algorithm-Based Approach for Investigating Catalyst Surface Morphology, **to be submitted**
- **Ghanekar, P.\***, Xie, P.\*, Choksi, T., Purdy, S., Miller, J., Greeley, J., Wang, C., Dispersed Ceria-Supported Copper Catalysts for Room Temperature Direct NO Reduction, **to be submitted**
- Purdy, S. C.\*, **Ghanekar P.\***, et al. [Origin of Electronic Modification of Platinum in a Pt 3 V Alloy and Its Consequences for Propane Dehydrogenation Catalysis. ACS Appl. Energy Mater. 3, 1410–1422 \(2020\).](#)
- **Ghanekar, P.**, Kubal, J., Cui, Y., Mitchell, G., Delgass, W., Ribeiro, F., Greeley, J., [Catalysis at Metal/Oxide Interfaces: Density Functional Theory and Microkinetic Modeling of Water Gas Shift at Pt/MgO Boundaries. Top. Catal. \(2020\).](#)

## CONFERENCE PRESENTATIONS

• <b>Pushkar Ghanekar</b> , Jeffrey Greeley, <i>AIChE Annual Meeting, Virtual</i>	November 2020
• <b>Pushkar Ghanekar</b> , Jeffrey Greeley, <i>North American Catalysis Society Meeting, Chicago (IL)</i>	June 2019
• <b>Pushkar Ghanekar</b> , Jeffrey Greeley, <i>AIChE Annual Meeting, Pittsburgh (PA)</i>	November 2018
• <b>Pushkar Ghanekar</b> , Jeffrey Greeley, <i>Purdue Graduate Student Organization Symposium (Poster)</i>	2018, 2019
• <b>Pushkar Ghanekar</b> , Jeffrey Greeley, <i>SUNCAT Stanford Summer School (Poster), Stanford (CA)</i>	2017

## ADDITIONAL INFORMATION

- **Awards:**  
AIChE CRE Division Meeting Grant Award (2020), Bill Murray Fellowship (CISTAR Fellowship 2020), K.C. Chao and Jiun Chao Graduate Education Endowment (AIChE Dept Travel Award, 2018), Ratan Tata Engineering Endowment (Merit-based educational scholarship, 2013-2016)
- **Language:** Hindi (native), Marathi (native), English (fluent), Spanish (basic)
- **Interests:** Cooking, Baking, Cycling, Gaming, Running, Squash