

# PUSHKAR G. GHANEKAR, Ph. D. Candidate

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## PROFESSIONAL SUMMARY

Chemical engineering Ph.D. candidate working on developing multi-scale catalyst models that capture the essential structure-function properties of the real-world catalyst through a combination of first-principles based modeling algorithms and deep learning; investigating design rules enabling the prediction and synthesis of next-generation (electro)catalysts. My goal is to function at the interface of industry/business functions and cutting-edge data analytics, deriving intellectual and economic value, and fueling innovation.

## EDUCATION

### Ph.D. in Chemical Engineering (Bill Murray CISTAR Fellow)

2016 – Ongoing

Purdue University (West Lafayette, Indiana)

Advisor: Prof. Jeffrey Greeley

GPA: 3.87/4.0

(Anticipated graduation: Summer 2021)

### B.E. in Chemical Engineering

2012 – 2016

Institute of Chemical Technology (Mumbai, India)

GPA: 9.17/10.0 (First Class with Distinction, Ranked 5<sup>th</sup> in a class of 85)

## SKILLS AND TECHNOLOGIES

**Programming languages:** Python (10+ years), HTML/CSS (2+ years), C (1 year), JavaScript (<1 year)

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

**Technologies:** PyTorch, Dask, RAPIDS.AI, Tensorflow+Keras, MATLAB, VASP, Aspen plus, Adobe Photoshop, Blender

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

## ACADEMIC PROJECTS

### PhD in Chemical Engineering

2016 – Ongoing

- **Thesis topic:** Investigation of morphology and functioning of multi-component catalytic interfaces using first-principles calculations
  - **Machine-learning aided acceleration of catalyst modeling using local environment-based crystal graph convolutional network** for oxygen-based electrocatalytic reactions
  - **Ab-initio thermodynamic and kinetic analysis** for multi-functional Pt/MgO for water-gas shift reaction
  - **Grand-canonical genetic algorithm-based toolkit** to assess metal-oxide phase stability (*in collaboration with Hennig group, University of Florida*)
- **React/flask-based web tool** for lab-scale hazard evaluation and risk assessment (*in collaboration with CISTAR and Purdue Process Safety and Assurance Center*)

### B.E. in Chemical Engineering

2012 – 2016

- **Senior Design Project:** Techno-economic feasibility analysis for production of 20,000 TPA of ortho-cresol via Green route
- Python-based option pricing using real-time stock market data
- Educational tool for web-scraping online thermodynamic data-tables

## INDUSTRY INTERSHIPS

### Research and Development Intern – Dow Chemical Company, Lake Jackson (Texas, USA)

June - August 2020

Apply AI and machine learning techniques to troubleshoot complex manufacturing problems and develop data analytics technologies to address emerging R&D and manufacturing opportunities

### Process Engineering Intern – Black and Veatch, Mumbai (India)

May - July 2015

Designing and optimization of proprietary LNG liquefaction unit

### Research and Development Intern – Hetero Drugs, Bengaluru (India)

June - August 2013

Scheduling chemical engineering operations for manufacturing API and involved in pilot plant scale-up

## RESEARCH PUBLICATIONS

- 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, **in preparation**
- **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, **in preparation**
- 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. \(2020\).](#)

## TEACHING & 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

## LEADERSHIP AND SERVICE

- Murdock Elementary Teaching Volunteer** 2017 - Present  
Teaching basic scientific concept to local school's third grade science club
- Purdue Catalysis Center Webmaster** 2018 - Present  
Responsible for designing, modifying, and maintaining Purdue Catalysis Center website [\[link\]](#)
- CISTAR-SURF Undergraduate Mentor** May 2019  
Taught fundamentals of high-performance computing, using python and bash, to setup production quality electronic structure calculations based on DFT
- CISTAR-SURF Highschool Teacher Mentor** May 2018  
Assisted 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.
- First-year Representative (Graduate Student Organization)** 2017 - 2018  
Represent the incoming cohort of first-year graduate students. Organize mentor-mentee program and miscellaneous activities targeted to make the graduate school transition seamless
- Purdue Cycling and Triathlon club member** 2017 - Present  
Responsible for organizing training rides, bike route planning, and volunteer recruitment for domestic race events
- Citizens' Climate Lobby (Lafayette Chapter) volunteer** 2019 - Present
- Technical Head and Core Organizing Team Member (Vortex 2014, Institute of Chemical Technology)** 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.

## CONFERENCE PRESENTATIONS

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

## ADDITIONAL INFORMATION

- **Awards:** 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, Running, Squash