

# PUSHKAR G. GHANEKAR, Ph. D. Candidate

G060C, Forney Hal of Chemical Engineering, 480 Stadium Mall Drive, Purdue University, West Lafayette, IN 47907

Email: pghaneka@purdue.edu

Phone no: +1 (646) 678-6435



## PROFESSIONAL SUMMARY

*Chemical engineering Ph.D. candidate working on building an atomistic-level understanding of catalyst functioning for industry-relevant reactions. Using a combination of multi-scale modeling algorithms, primarily based on Density Functional Theory, and chem-informatics tools to develop design rules allowing for the prediction and development of next-generation catalysts.*

## EDUCATION

### PhD in Chemical Engineering

Purdue University (West Lafayette, Indiana)

Advisor: Prof. Jeffrey Greeley

GPA: 3.86/4.0

(Anticipated graduation: Summer 2021)

2016 – Ongoing

### B.E. in Chemical Engineering

Institute of Chemical Technology (Mumbai, India)

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

2012 – 2016

## SKILLS AND TECHNOLOGIES

**Programming languages:** Python (8+ years), html/css (2+ years), C (1 year), JavaScript (<1 year)

**Recent Coursework:** Neural Networks and Deep Learning, Improving Deep Neural Networks, Convolutional Neural Networks, Data science in ChE,

**Technologies:** PyTorch, MATLAB, VASP, GPAW, ASE, Aspen plus, Flask, Final Cut Pro, Adobe Photoshop, Blender

**Tools/packages:** numpy, pandas, scipy, matplotlib, scikit-learn, selenium, beautifulsoup, git, emacs, bash

## PROJECTS

### PhD in Chemical Engineering

- **Thesis topic:** *Investigation of morphology and functioning of multi-component catalytic interfaces using first-principles calculations*
  - **Investigation of multi-metallic alloys using local environment-based crystal graph convolutional network** for oxygen-based electrocatalytic reactions
  - **High throughput screening** of perovskite-supported platinum catalyst for water-gas shift reaction
  - **Microkinetic modeling and dopant screening** for multi-functional Pt/MgO for water-gas shift reaction
  - **Ab-initio thermodynamic and kinetic analysis** of atomically dispersed catalyst on ceria for NO decomposition (*in collaboration with Wang group, John Hopkins University*)
  - **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*)

2016 – Ongoing

### B.E. in Chemical Engineering

- **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** based on Black-Scholes-Merton option pricing model
- **Educational tool for web-scraping online thermodynamic data-tables** and model thermodynamic equation of state

2012 – 2016

## LEADERSHIP AND SERVICE

### Murdock Elementary Teaching Volunteer

Teaching basic scientific concept to local school's third grade science club

2017 - Present

### Purdue Catalysis Center Webmaster

Responsible for designing, modifying, and maintaining Purdue Catalysis Center website [\[link\]](#)

2018 - Present

### CISTAR-SURF Undergraduate Mentor

Taught fundamentals of high-performance computing, using python and bash, to setup production quality electronic structure calculations based on DFT

May 2019

|   |                |
|---|----------------|
| <b>CISTAR-SURF Highschool Teacher Mentor</b>  | 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.                      |                |
| <b>First-year Representative (Graduate Student Organization)</b>  | 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.  |                |
| <b>Purdue Cycling and Triathlon club member</b>   | 2017 - Present |
| Responsible for organizing training rides, bike route planning, and volunteer recruitment for domestic race events  |                |
| <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 EXPERIENCE

|   |             |
|---|-------------|
| • 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.**, V.S. Chaitanya Kolluru, 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. \(2020\).](#)

## CONFERENCE PRESENTATION

|   |               |
|---|---------------|
| • <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          |

## INTERNSHIPS

|   |                    |
|---|--------------------|
| <b>Research and Development Intern – Dow Chemical Company, Lake Jackson (Texas, USA)</b>  | 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 |                    |
| <b>Process Engineering Intern – Black and Veatch, Mumbai (India)</b>  | June - August 2015 |
| Designing and optimization of proprietary LNG liquefaction unit   |                    |
| <b>Research and Development Intern – Hetero Drugs, Bengaluru (India)</b>  | June - August 2014 |
| Scheduling chemical engineering operations for manufacturing API and involved in pilot plant scale-up   |                    |

## ADDITIONAL INFORMATION

- **Awards:** 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