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

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 *2016 – Ongoing*
Purdue University (West Lafayette, Indiana)
Advisor: Prof. Jeffrey Greeley
GPA: 3.86/4.0
(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 5th in 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, scipy, matplotlib, scikit-learn, selenium, beautifulsoup, git, emacs, bash

PROJECTS

PhD in Chemical Engineering *2016 – Ongoing*

- **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)*

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

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.

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

- **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*

INTERNSHIPS

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) *June - August 2015*

Designing and optimization of proprietary LNG liquefaction unit

Research and Development Intern – Hetero Drugs, Bengaluru (India) *June - August 2014*

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

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