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-functional 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 5th 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 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

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).

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

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