PUSHKAR G. GHANEKAR, Ph. D. Candidate

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PROFESSIONAL SUMMARY

Curious, open-minded, and driven, Chemical engineering Ph.D. candidate developing a molecular-level understanding of catalysts through a combination of chemistry, physics, and machine-learning. Functioning in cross-disciplinary collaboration, my primary focus is building computational catalyst models that capture essential properties of the real-life catalyst. My work is directed towards improving fuel-cell technologies as a sustainable alternative to fossil fuel resources for meeting future energy demands. My career goal is to be part of a multi-disciplinary team in a data-driven ethos, digitizing the traditional R&D process using AI/ML methods. To work at the interface of industry/business functions, 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)

SKILLS AND TECHNOLOGIES

Programming languages: Python (10+ years), Bash (4+ 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: High-Performance Computing (CPU/GPU), PyTorch, Dask, Nvidia RAPIDS.AI, Tensorflow, MATLAB, VASP/GPAW, Aspen plus, Adobe Photoshop, Blender
Tools/packages: NumPy, Pandas, Matplotlib, Scikit-learn, Selenium, Beautifulsoup, git, emacs

ACADEMIC PROJECTS

Ph.D. in Chemical Engineering *2016 – Ongoing*

- **Thesis topic:** *Investigation of morphology and functioning of multi-component catalytic interfaces using first-principles calculations*
  - **Machine-learning based software for the acceleration of catalyst modeling using local environment-based graph convolutional network:** Gives the ability to screen complex surface catalyst model under reaction conditions
  - **Engineering active-site and investigating reaction mechanism:** Proposed new active site models that improved the understanding for Water-gas shift and NOx decomposition
  - **Grand-canonical genetic algorithm-based toolkit** to generate complex catalyst models hitherto deemed challenging *(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
- An 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 multi-variate data analysis 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:**
  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, Running, Squash