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PROFESSIONAL SUMMARY

As a Senior Research Advisor at Eli Lilly and Company, I currently lead an AI-driven drug discovery project and have extensive experience in early-stage discovery across various therapeutic areas and molecular modalities. In particular, I have expertise in data science, cheminformatics, high-throughput screening, and chemistry-aware AI model development. I also bring expertise in leading successful multi-disciplinary research collaborations.

My passion is to harness data and AI to create better medicines faster, ultimately improving the quality of lives worldwide.

SKILLS AND TECHNOLOGIES

Project management:
Agile workflow and scrum, Medicine discovery project management: chemistry-biology collaboration, assay flow scheme optimization, target exploration and enablement.

Computer-Aided Drug Design + Cheminformatics:
Cheminformatics, Hit expansion from HTS, fragment and substructure search (SMARTS, SMIRKS, Protocolbuffers), Library design (fragment and reaction-based enumeration), R-group analysis, DFT simulations (VASP, GPAW), Lead optimization (multi-parameter optimization), retrosynthesis analysis, molecular docking.

Technologies:
Large Language Models (LLMs) for chemistry, Artificial Intelligence (AI) methods, High-Performance Computing (CPU/GPU), Data management systems (MongoDB, SQL), REST API, Data visualization (matplotlib, seaborn, tableau), Docker, GitOps, AWS (with Kubernetes)

Tools:
Langchain, PyTorch (+Geometric), Tensorflow, Networkx, XGBoost, Dask, RDkit, LillyMol, Scikit-Learn, PyData Stack, CuPy, SQLAlchemy, Pandas, Flask

Data Science / Modeling Skills:
Graph neural networks, Generative models (VAE, LSTM), Classification algorithms (XGBoost, SVM), Bayesian optimization / Active learning, Dimensionality reduction (PCA, diffusion maps), Multivariate analysis (PLS-DA, PCA, Batch evolution modeling), Web scraping (selenium, beautifulsoup)

Recent Coursework:
AI Agents using LLM (deeplearning.ai), Prompt Engineering for Developers (deeplearning.ai), Medicinal Chemistry and Biology in Drug Discovery (Drew University), Intro to Cloud computing, Bayesian Statistics, Deep learning specialization (deeplearning.ai), Data Science in Chemical Engineering

INDUSTRY EXPERIENCE

Sr. Advisor – Chemistry, Eli Lilly and Company, Indianapolis (Indiana, USA) September 2023 - Present

- Project lead on antibacterial drug discovery project in collaboration with OpenAI (Press Release)
- Lead Drug Discovery AI agent platform development with a cross functional team of software engineers and research scientist
- Lead target selection, enablement, and drug discovery project in the antibacterial space.
- Contribute to computational modeling of medicine discovery in neurodegenerative and obesity targets using state-of-the-art cheminformatics and digital chemistry techniques.
- Facilitate adoption of state-of-the-art (generative) AI molecular design tools by cross-functional collaboration with medicinal chemistry, pharmacology, and structural biology
- Identify and collaborate with external research groups in leading artificial intelligence and reaction informatics, facilitate research projects to adopt leading edge research

Advisor – Chemistry, Eli Lilly and Company, Indianapolis (Indiana, USA) October 2021 - September 2023

- Part of computational modeling drug hunter team working on small molecule early stage portfolio projects with primary focus on bifunctional degraders, non-peptide agonists, and molecular glues
- Contributing to reaction informatics, route design, generative AI method development to accelerate design-make-test cycle times

Chemometric & AI Intern, Dow Chemical Company, Lake Jackson (Texas, USA) June 2020 - August 2020

High throughput small-molecule screening (Cheminformatics, Core R&D):

- Designed, developed, and deployed ML model for small molecule discovery – generative and regression model

- Scaled-up model inference capabilities resulting in a 30-fold improvement in compute time, increasing the ability to screen potential molecules from millions to billions.

Anomaly detection model & root-cause analysis (Manufacturing & Engineering Analytics):
- Performed multivariate time-series analysis (PCA, PLS-DA, and Batch Evolution Modeling) to troubleshoot complex manufacturing problems in collaboration with plant engineers.
- Proposed key process variables driving the manufacturing process upsets.
- Build a detection model (Variational Autoencoder) to identify process anomalies at least 12 hours in advance, improving overall plant reliability & safety.

EDUCATION

Ph.D. in Chemical Engineering 2016 – 2021
Purdue University (West Lafayette, Indiana) | GPA: 3.87/4.0
B.E. in Chemical Engineering 2012 – 2016
Institute of Chemical Technology (Mumbai, India) | GPA: 9.17/10.0 (First Class with Distinction)

RESEARCH EXPERIENCE

Graduate Research Assistant (Bill Murray CISTAR Fellow) 2016 – Present

Advisor: Prof. Jeffrey Greeley
Thesis: Investigation of Morphology and Functionality of Multi-Component Catalyst using First-Principles and Machine-Learning
8 Peer-reviewed publications | 2 Open-source python packages | 1 Online-tool

1. **Physics-inspired machine learning model for high-throughput catalyst screening**
   - Accelerated virtual screening of complex catalyst surface models to investigate complicated reaction dynamics.
   - First-ever extension of Graph Neural Networks to encode complex catalyst surfaces.
   - Identified new surface representation aiding better understanding of electrochemical surface morphologies.
   - Designed an active-learning strategy to enhance model learning and sampling.
   - Pioneered machine-learning application in the research group.

2. **Genetic algorithm for building catalyst interfacial models**
   - Genetic algorithm to generate and understand complex surface chemical transformations
   - First-of-its-kind algorithm to generate metal/oxide interfacial models that capture necessary chemical complexity. Developed the geometric lattice matching code to create the said models systematically.
   - Work in collaboration with the University of Florida

3. **Catalyst active-site engineering, statistical modeling, and investigating reaction mechanism:**
   - Collaborated with the experimental group to design experiments and propose design rules for building better catalysts through novel catalyst active-site models, free-energy analysis, and rigorous microkinetic modeling
   - Built a random forest model to predict the main features dictating the catalyst stability resulting in an improved understanding of the chemical process
   - Reactions studied: H_2 production, shale gas processing, and low-temperature Automotive Emission Control processes
   - Work in close collaboration with research groups at Purdue, John Hopkins, Maryland, and Argonne National Lab

4. **Online lab-scale hazard evaluation and risk assessment tool:**
   - Open-source tool to compile and scrutinize hazards-related information before performing experiments.
   - Proposed, planned, and co-developed logic for operational hazard evaluation workflow, chemical property estimation, and datasheet parsing algorithm.
   - Led the beta-testing effort amongst research groups in partner universities.
   - Work in collaboration with CISTAR (NSF-funded engineering research center), Corteva Agriscience, and Purdue Process Safety and Assurance Center.

LEADERSHIP AND SERVICE

Community Outreach Chair (American Chemical Society – Indianapolis Chapter) 2021 - Present
Led planning and execution of outreach events for the Indianapolis Chapter of the American Chemical Society. Focus on encouraging STEAM education amongst underprivileged groups. Work with River cleanup group to conduct periodic clean-up and charity drives.

Planning committee member (New Employee Acceleration & Training) summit 2021 - 2022
Organizing Committee of the New Employee Acceleration & Training Summit – a 1st of it's kind learning, training, mentoring, and networking event to connect new scientists across pillars and geographies throughout Eli Lilly and Company's Discovery Chemistry.

Murdock Elementary Teaching Volunteer 2017 - 2022

Teaching introductory science and math concepts to third-grader science club at local elementary school

Purdue Catalysis Center Webmaster 2018 - 2021
Responsible for designing and maintaining the Purdue Catalysis Center website – A central location for all heterogeneous catalysis-related research at Purdue Chemical Engineering. [link]

CISTAR-SURF Undergraduate Mentor May 2019
Taught fundamentals of high-performance computing, python, bash, and setup electronic structure calculations based on DFT

CISTAR-SURF Highschool Teacher Mentor May 2018
Advised a nationwide cohort of high-school teachers on developing STEM courses focused on lab-scale reactions, high-performance computing, coding, and essential algorithm development in the school curricula. Built a python-based GUI to teach simple chemical reaction design.

First-year Representative (Graduate Student Organization) 2017 - 2018
Represent the incoming first-year graduate students. Organized mentor-mentee program and activities targeted to make the graduate school transition seamless for international students

Purdue Cycling and Triathlon club member 2017 – 2021

Citizens' Climate Lobby (Lafayette Chapter) volunteer 2019 – 2022

Technical Head and Core Organizing Team Member (Vortex 2014, Institute of Chemical Technology) 2014 - 2015
Designed, built, and managed the event website. Organized the IDP (Industry Defined Problem), the conference's main event, with a total participation of 1500 students. Increased event participation by 15% compared to the previous two years. Lead Designer involved in designing festival merchandise and apparel.

TEACHING AND MENTORING EXPERIENCE

- Medical Innovation Hub Mentor (Eli Lilly & Company, USA): 3 mentees — Spring 2023 - Present
- Visiting professor for Cheminformatics (Sophia College, Mumbai) — Fall 2022 - Present
- Visiting Ph.D. Thesis advisor (Institute of Chemical Technology, Mumbai) — Summer 2023 - Present
- Mentor summer replacement (2) and post-doctoral employees (2) — Spring 2022 – Present
- Data science project mentor and judge (The Erdős Institute) — Fall 2021& Spring 2023
- Data Analytics and Machine Learning REU Mentor and Judge (CISTAR-Purdue DataCamp) — Summer 2021
- Onboarding and mentoring new graduate students in the research group — Fall 2018 – Spring 2022
- Coding and research mentors for High School teachers (CISTAR-Purdue) — Summer 2019
- 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 [Google Scholar]

- Deshmukh, G; **Ghanekar, P**; Greeley, J; A combined first principles and data-driven computational framework to analyze the surface structure, composition, and stability of alloy catalysts, ChemRxiv (2024)
- Deshmukh G, Wichrowski NJ, Evangelou N, **Ghanekar P,** Deshpande S, Kevrekidis IG, et al. Active Learning of Ternary Alloy Structures and Energies. NPJ Computational Materials, 2024.
- **Ghanekar, P.,** Siddharth Deshpande, and Jeffrey Greeley. "Adsorbate chemical environment-based machine learning framework for heterogeneous catalysis." Nature Communications 13.1 (2022): 1-12. (Purdue News Article)
- Ezenwa, S., Talpade, A. D., **Ghanekar, P.**, Joshi, R., Devaraj, J., Ribeiro, F. H., & Mentzer, R. (2022). Toward Improved Safety Culture in Academic and Industrial Chemical Laboratories: An Assessment and Recommendation of Best Practices. *ACS Chemical Health & Safety*, *29*(2), 202-213.
- Talpade, A.*, **Ghanekar, P.*** et al., Promoting a Safe Laboratory Environment Using the Reactive Hazard Evaluation & Analysis Compilation Tool (RHEACT), ACS Chemical Health & Safety (2021)
- 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., *et. al.* Catalysis at Metal/Oxide Interfaces: Density Functional Theory and Microkinetic Modeling of Water Gas Shift at Pt/MgO Boundaries. Top. Catal. (2020).

Manuscript in preparation (draft available upon request):

- Verma N., Ru X., Younkunas M., **Ghanekar P.,** Practical AI-Generative Design to Augment and Accelerate Early-Stage Drug Discovery (in preparation)
- **Ghanekar, P.*,** Xie, P.*, *et. al.,* Ceria Supported Copper Dimers for Near-Ambient-Temperature Decomposition of NO, **to be submitted**
- V.S. Chaitanya Kolluru, **Ghanekar, P.** *et al.*, Grand Canonical Evolutionary Algorithm-Based Approach for Investigating Catalyst Surface Morphology, **under review**

Patent:

- US 63/425,751 (Small molecule chemical space for high-value portfolio target in Diabetes space)
- US 30930_US_PRI (Small molecule chemical space for high-value portfolio target in Diabetes space)

Journal reviewing:
- Journal of Chemical Information and Modeling (2)
- Nature Communications (2)
- Molecular Informatics (4)

CONFERENCES AND PRESENTATIONS

- **Pushkar Ghanekar,** Ian Watson,et. al., LillyMol : Cheminformatics toolkit for precise and fast structure search, chemical transforms, and other cheminformatics tasks, ACS Spring 2024 — March 2024
- Gaurav Deshmukh, Noah Wichrowski, Pushkar Ghanekar, et. al., Active Learning Workflow for Discovery of Stable Ternary Alloys from Binary Alloy Data, AIChE Fall 2023 — November 2023
- **Session Co-chair:** Catalysis on Low Dimensional Materials II, *AIChE Annual Meeting, Virtual* — November 2020
- **Pushkar Ghanekar**, Jeffrey Greeley, *AIChE Annual Meeting, Virtual* — June 2019
- **Pushkar Ghanekar**, Jeffrey Greeley, *North American Catalysis Society Meeting, Chicago (IL)* — November 2018
- **Pushkar Ghanekar**, Jeffrey Greeley, *AIChE Annual Meeting, Pittsburgh (PA)* — 2018, 2019
- **Pushkar Ghanekar**, Jeffrey Greeley, *Purdue Graduate Student Organization Symposium (Poster)* — 2017
- **Pushkar Ghanekar**, Jeffrey Greeley, *SUNCAT Stanford Summer School (Poster), Stanford (CA)*

ADDITIONAL INFORMATION

Professional Society memberships:
- American Chemical Society
- American Institute of Chemical Engineers

Awards:
- Lilly Research Award Program funding with CalTech (Fall 2023)
- Top 100 Lilly Innovator Award (recognized across the organization), Fall 2023
- Lilly Innovator Award (Fall 2022 and Spring 2023)
- 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)