

Kaustubh Sawant

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Professional Summary:

Chemical Engineering PhD candidate with proven experience in software engineering, materials modeling, machine learning, and data analytics. Seeking positions to work in a collaborative and diverse team while fueling sustainable solutions for a better future.

Education:

PhD in Chemical Engineering, Purdue University, West Lafayette, IN **2018-March 2023(Expected)**

GPA: 3.82/4.00

Advisor: Prof. Jeffrey Greeley

Research Topic: Elucidating Structure-Property Relationships at Metal-Metal Oxide Interfaces for Catalysis.

B.E in Chemical Engineering, Institute of Chemical Technology, Mumbai, India **2014-2018**

GPA: 9.36/10.00, GRE: 329/340

Skills and Technical Expertise:

Programming Languages: Shell/Bash, Python, HTML/CSS, Excel/VBA, MATLAB

Modeling/Data Science Tools:

- o Density Functional Theory Simulations - VASP, GPAW, QBOX
- o Molecular Dynamics Simulations - VASP, LAMMPS, ASE
- o Process Simulations - Aspen plus, Pyomo
- o AI/ML - TensorFlow, PyTorch, Scikit-learn, Pandas, Networkx, wandb, Sympy
- o Miscellaneous Modelling tools – Pymatgen, Matminer, ASE

Technologies: High Performance Computing (CPU/GPU), Git

Recent Courses:

Deep learning specialization (Deeplearning.ai), Statistical machine learning (Purdue CS578), Atomistic view of materials: Modeling and simulations (Purdue ME697), Advanced modeling for catalysis (Purdue ChE 697)

Research Experience:

PhD Candidate, Purdue University, West Lafayette, IN **2018-Present**

Thermodynamic Formulism for Surface Science Experiments

- o Developed a novel framework to make *ab initio* thermodynamic hull diagrams for ultra-high vacuum (UHV) surface science experiments including atomic layer deposition experiments.
- o Proposed a thermodynamic scheme to bridge the gap between UHV experiments and industrially relevant reaction conditions.

Method Development [[github.itap.purdue.edu/sawantk](https://github.com/itap.purdue.edu/sawantk)]

- o Developed lattice matching algorithm to enumerate non pseudomorphic film structures.
- o Developed an active deep learning method for simulating metal-water interfaces.
- o Developed non mean field cluster expansion and microkinetic model calculator using Sympy and Networkx.

Universal Properties of Metal Supported Oxide Films

- o Developed models to accurately predict the formation of metal supported metal oxide films.
- o Proposed a new bonding model to explain deviations from bond order conservation principles.
- o Worked in close collaboration with experimental groups at Purdue University to develop prediction tools for overlayer formation in strong metal support interaction.
- o Proposed a theory to explain the change in the chemical properties of key intermediates due to the presence of the thin film oxides using charge transfer.

Discovery of New Materials for Oxygen Reduction Reaction

- o Predicted the existence of stable single atom and 2d metal oxide dopants that can enhance the activity and stability of Pt group catalysts for oxygen reduction reaction using explicit solvation models.
- o Developed a local strain-based model to explain the enhancement in activity.

Group Responsibilities

- o Led research group in upkeep of atomic calculation codes on the Purdue Community Clusters (RCAC).
- o Prepared detailed documents to ensure transfer of good engineering and coding practices to onboard new graduate students in the research group.

Professional Experience:

Summer Design Intern, Jacobs Engineering (Fortune 500), Mumbai, India

Summer 2017

- o Reduced ~2hrs of manual work by developing an automated system to optimize chemical separators and tanks using a combination of Excel and VBA.
- o Performed systematic check of process and instrumentation diagrams to ensure consistency.

Summer Intern, Vanguard Industrial Hygiene Laboratory, Pune, India

Summer 2016

- o Collaborated with Certified Industrial Hygienist Subhash Nikam to mitigate volatile solvent at Lupin Research Park, Pune, India.
- o Prepared report identifying causes for solvent leaks and provided strategies for safe handling of solvents.

Publications: (* Co first author)

- o Gao, J*.; **Sawant, K. J*.**; Miller, J. T.; Zeng, Z.; Zemlyanov, D.; Greeley, J. P.; Structural and Chemical Transformations of Zinc Oxide Ultrathin Films on Pd(111) Surfaces. ACS Appl. Mater. Interfaces 2021, 13 (29), 35113–35123.
- o **Sawant, K. J.**; Zeng, Z.; Greeley, J. P.; Universal properties of metal-supported oxide films from linear scaling relationships: Elucidation of Strong Metal Support Interactions. (*In peer review*)

In preparation: (*Drafts available on request*)

- o **Sawant, K. J*.**; Gao, J*.; Miller, J. T.; Zeng, Z.; Zemlyanov, D.; Greeley, J. P.; Tuning adsorption properties of metals through metal-hydroxide interaction.
- o Smith, J*.; **Sawant, K. J*.**; Zeng, Z.; Wu, J.; Greeley, J. P.; Gao, W.; Chemistry under atomic resolution microscopy – visualizing reactions by intermediates by tracking the behaviors of atoms.
- o **Sawant, K. J.**; Zeng, Z.; Greeley, J. P.; Stability of metal oxides on metal nanoparticles and its impact on oxygen reduction reaction.

Conference Presentations: (* Presenting Author)

- o **Sawant, K. J*** et al, *AICHE Annual Meeting* **2022**
- o **Sawant, K. J*** et al, *Purdue ChE Symposium* **2022**
- o **Sawant, K. J.**, Greeley, J.P* et al, *ACS Fall Meeting* **2022**
- o **Sawant, K. J***, Greeley, J.P et al, *NAM Meeting (Poster)* **2022**

- o **Sawant, K. J**, Greeley, J.P* et al, *ACS Spring Meeting* 2022
- o **Sawant, K. J*** et al, *AICHE Annual Meeting, Virtual* 2020
- o **Sawant, K. J*** et al, *SUNCAT Stanford Summer School* 2020

Teaching Experience:

- o **DFT Coding Assistant**, Advanced Modeling for Catalysis (ChE 697) *Spring 2022*
- o **Teaching Assistant**, Design and Analysis of Processing Systems (ChE 450) *Spring 2021*
- o **Teaching Assistant**, Chemical Engineering Thermodynamics (ChE 211) *Fall 2019*

Awards:

- o Best Oral Presentation, Catalysis and Reaction Engineering, Purdue ChE Symposium 2022
- o K.C. Chao and Jiun Chao Graduate Education Endowment 2020

Extracurricular Experience:

- Organizing Coordinator and Webmaster**, Purdue Catalysis Center, West Lafayette, IN *2021-Present*
- o Organized weekly scientific talks and presentations to nurture collaborative work in catalysis at Purdue.
- o Improved and maintained the Purdue Catalysis Center website to highlight research and professional profiles of graduate students.

- Murdoch After School Program Volunteer**, Purdue ChE GSO, West Lafayette, IN *2021 -Present*
- o Taught science lessons to 3rd and 4th grade students at the Murdock elementary school, Lafayette.

- Overall Head and Secretary**, Vortex ICT, Mumbai, India *2016-2017*
- o Led a team of 100+, planned and organized Vortex, ICT's technical festival.
- o Member of the ICT students' council and responsible for ensuring collaboration between industry and students.

Sports Activities:

- o Represented college for lawn tennis and soccer.
- o Black Belt in Karate (2012)

Languages: English (fluent), Marathi (native), Hindi (native)

References:

PhD Advisor: Prof. Jeffrey Greeley (jgreeley@purdue.edu)

Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

Experimental Collaborator and PhD Committee Member: Prof. Jeffrey Miller (jeffrey-t-miller@purdue.edu)

Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

PhD Committee Member: Prof. Rajamani Gounder (rgounder@purdue.edu)

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