VAIDISH SUMARIA

1811 S Bentley Ave., Los Angeles, CA 90025

+1(412)-403-1313 ∘ vsumaria@g.ucla.edu ∘ linkedin.com/in/vaidishsumaria/ ∘ website:vsumaria.github.io/

EDUCATION

University of California Los Angeles *Aug. 2018-Aug. 2022*
Ph.D. Chemical Engineering GPA: 4.0
Carnegie Mellon University, Pittsburgh *Jun. 2016-Dec. 2017*
MS Chemical Engineering GPA: 4.0
University of Petroleum and Energy Studies, Dehradun, India *Jun. 2012-May 2016*
B.Tech. Chemical Engineering with Specialization in Refining and Petrochemicals (Silver Medalist) GPA: 3.57
Relevant Graduate Courses: AI & Machine Learning, Neural Networks and Deep Learning, Data Management and Statistical Computing, Statistical Thermodynamics, Mathematical Modeling, Statistical Thermodynamics, Electrochemical Energy Systems, Industrial Chemical Technology, Interface Engineering.

TECHNICAL SKILLS

Programming: Python, Matlab, C++, SAS, R, Scikit-Learn, PyTorch
Modeling: VASP, GPAW, Atomic Simulation Environment, LAMMPS, Comsol, Aspen Plus
Experimental: Gas Chromatography, Temperature Programmed Desorption, BET Surface Area Analyzer

INDUSTRIAL EXPERIENCE

Computational Chemistry Intern, Phaseshift Technologies Inc. *Jan. - Sep. 2021*

- Created a database for Bulk Metallic glass (BMG) alloy properties to train machine learning models for mechanical property prediction
- Developed framework for creating interatomic potentials for BMG with different compositions for rapid exploration.
- The potentials were used to estimate the liquid and glass transition temperatures.

Intern, Reliance Industries Limited, Patalganga, India *Jun.-Jul. 2014*

- Designed Prefractionation column for Para-xylene unit to combine the operations of two columns.
- Developed Aspen model had the Naphtha feed separated into the lighters (C1-C6), the heaviers (C10 on-wards) and the heart-cut (C7-C9) was obtained from a side-stream with the required concentrations.

RESEARCH EXPERIENCE

Research Assistant, Sautet Lab, UCLA, USA *Aug. 2018- Present*

- Developed a C-O bond distance based energy correction for the DFT energies to solve "Pt/CO Puzzle".
- Using thermodynamic analysis, generated stability diagram to understand Pt-CO system in real reaction conditions.
- Developed High Dimensional Neural Network potential for the system to investigate surface reconstruction.
- Designed modified Grand Canonical Basin Hopping to efficiently explore configurations.

Research Assistant, Viswanathan Lab, CMU, Pittsburgh *Sep. 2017-Jul. 2018*

- Developed a rigorous framework to propagate uncertainty within thermodynamic catalytic activity-prediction models.
- Defined a computational measures: prediction efficiency and confidence values to quantitatively the correct energy descriptors for a given reaction scheme and degree of confidence in the predicted surface phase diagrams respectively.
- Studied electrochemical oxygen, hydrogen and chlorine evolution reactions: activity and selectivity predictions

Mitacs Globalinks Intern, University of Saskatchewan, Canada *Jun. 2017-Aug. 2017*

- Optimized fixed bed adsorption by functional polymers for the removal of refractory nitrogen species from bitumen derived gas oil. Effects of temperature and flow rates were also studied and used to develop a mathematical model.

Graduate Researcher, Gopalakrishnan Lab, UPES, India *Aug. 2013-Apr. 2014*

- Optimized the synthesis parameters of ZSM-12 catalyst for the direct conversion of n-Butane to iso-octane.
- Devised a seed assisted synthesis technique to avoid the use of expensive and toxic organic structure directing agents.

PUBLICATIONS

- CO organization at ambient pressure on stepped Pt surfaces: First principle modeling accelerated by neural networks. **Chem. Sci.**, 2021.
- Optimal packing of CO at high coverage on Pt(100) and Pt(111) surfaces, **ACS Catal.**, 2020.
- Maximal predictability approach for identifying the right descriptors for electrocatalytic reactions, **J. Phys. Chem. Lett.**, 2018, 9 (3), pp 588595.
- Quantifying Confidence in DFT Predicted Surface Pourbaix Diagrams and Associated Reaction Pathways for Chlorine Evolution, **ACS Catal.**, 2018, 8 (10), pp 90349042.
- Quantifying robustness of DFT predicted pathways and activity determining elementary steps for electrochemical reactions, **J. Chem. Phys.** 150, 041717 (2019).