Vaidish Sumaria

Graduate Researcher

+1-412-403-1313

vsumaria@andrew.cmu.edu

andrew.cmu.edu/∼vsumaria/

/in/vaidishsumaria/

Skills

Programming: Python, Matlab, C++, HTML(basic), LaTeX

Modeling Platform: Comsol, Aspen Plus, Aspen Plus Dynamics, APC Model builder, GAMS, HTRI, gPROMS

Experimental: Gas Chromatography, Temp. programmed Desorption, BET Surface Analyzer, Nitrogen Sulfur analyzer, Fixed Bed Reactors (pilot plant)

Courses

Graduate (CMU):

Electrochemical Energy Systems,
Advanced Thermodynamics,
Math Modeling of ChemE Processes,
Chemical and Reactive Systems,
Transport Phenomena,
Process Systems Modeling,
Industrial Chemical Technology

Undergraduate (UPES):

Heat Transfer,
Mass Transfer,
Fuild Mechanics,
Particulate Technology,
Chemical Thermodynamics,
Reaction Engineering,
Process Control,
Refining and Petrochemical Technology,
Natural Gas Engineering

Education

University of California, Los Angeles , CA — Aug. 2018 - Present
PhD student, Chemical Engineering

Carnegie Mellon University, Pittsburgh, PA — Aug. 2016 - Dec. 2017
Master of Science, Chemical Engineering
GPA: 4.0/4.0

University of Petroleum and Energy Studies, India — Jun. 2012 - May 2016
Bachelor of Technology, Chemical Engineering
GPA: 3.57/4 (Silver Medalist)

Research Experience

Understanding the restructuring of model metal catalysts in reactant gases
Prof. Philippe Sautet, University of California Los Angeles, Aug. 2017 - Present

- Understanding the general Trends for CO adsorption on metal surfaces as a function of coordination.
- Building DFT data base and training HDNNP for CO on Pt surfaces.
- Colaborating with *Prof. Feng Tao's* group at University of Kansas to develope a Mechanism for the CO induced restructuring for Pt starting from STM data

Understanding the Selectivity between ClER and OER on Rutile Oxides
Prof. Venkat Viswanathan, Carnegie Mellon University, Sep. 2017 - Jul. 2018

- Developed a method to quantify uncertainty in the scaling relations as a function of the descriptor.
- Currently working on propagating the variable uncertainty to create a generalized probabilistic Pourbaix diagram.

Self-Formed Catalysts using Electrochemical Lithiation
Prof. Venkat Viswanathan, Carnegie Mellon University, Aug. 2017 - Present

- Known electrode materials are tested for their potential to catalyze various electrochemical reactions.
- Electrochemical intercalation is used to tune the strain and electronic structure of the catalyst.

Quantification of Uncertainty in DFT derived Material Properties
Prof. Venkat Viswanathan, Carnegie Mellon University, Oct. 2016 - Sep. 2017

- Developed a rigorous framework to propagate uncertainty within thermodynamic activity-prediction models.
- Defined a new quantity Prediction Efficiency as a measure to quantitatively find the correct descriptor for a given reaction schemes.

Publications

- D. Krishnamurthy*, **V. Sumaria***, and V. Viswanathan. **Maximal predictability approach for identifying the right descriptors for electrocatalytic reactions** J. Phys. Chem. Lett., 2018, 9 (3), pp 588–595 (*Equal Contribution).
- **V. Sumaria**, D. Krishnamurthy, and V. Viswanathan. **Quantifying Confidence in DFT Predicted Surface Pourbaix Diagrams and Associated Reaction Pathways for Chlorine Evolution** ACS Catal., 2018, 8 (10), pp 9034–9042.
- D. Krishnamurthy, **V. Sumaria**, and V. Viswanathan. **Quantifying robustness of DFT predicted pathways and activity determining elementary steps for electrochemical reactions** J. Chem. Phys. 150, 041717 (2019).