Viswanath Pasumarthi

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- **Computational Scientist with over 10 years of experience in research**, specializing in modeling chemical physics across the fields of chemistry, electrocatalysis, materials science.
- **I have developed scientific software tools such as PyCD and CatEnergy**, combining my interest in programming with the goal of enabling scientific research.
- **I enjoy approaching challenging problems with curiosity and scientific understanding**, utilizing cutting-edge technologies to understand and solve emergent behaviors of physical systems across multiple scales.
- **My contributions to the field are recognized through 10 peer-reviewed publications** and prestigious awards, including the Gandhian Young Technological Innovation Award and the ACS CATL Travel Award (list available upon request).

EDUCATION

Ph.D., in Chemical Engineering   **Aug 2015 – May 2020**
University at Buffalo, The State University of New York   GPA: 3.6/4.0
Master of Technology in Chemical Engineering   **Jul 2012 – May 2014**
Indian Institute of Technology, Guwahati, India   GPA: 9.2/10.0
Bachelor of Technology in Chemical Engineering   **Jul 2008 – Jun 2012**
National Institute of Technology, Calicut, India   GPA: 7.2/10.0

RESEARCH EXPERIENCE

Postdoctoral Research Associate, Purdue University   **Aug 2023 – Present**
- **Conducted extensive Ab-Initio Molecular Dynamics** simulations for low-temperature electrocatalytic alkane dehydrogenation on Pt-based catalysts to understand reaction mechanisms and thermodynamic properties.
- **Elucidated the effects of solvation and surface charge** on adsorption and reactivity of alkane dehydrogenation on the Pt surface.

Postdoctoral Scholar, SUNCAT Center for Interface Science, SLAC   **Aug 2020 – July 2023**
- **Developed CatEnergy**, an open-source Python tool automating free energy computations in catalysis, integrating with **Catalysis-Hub** to enable scientific data retrieval and reproducible workflows and **CatMAP** for microkinetic modeling.
- **Led collaborative efforts** to compare explicit, implicit, and hybrid solvation models, elucidating solvation and electric field effects at the electrode/electrolyte interface to guide model selection for CO_2 electroreduction on copper catalysts.
- **Conducted one of the first systematic solvation benchmarking studies**, showing that larger, polar intermediates are especially sensitive to these effects in the reduction to C_1, C_2 products.

- **Characterized catalytic activity and selectivity** of CO_2 reduction on multi-faceted crystalline CuNPs using potential-dependent DFT and microkinetic modeling, identifying facet-specific selectivity towards C_1 and C_2 products and highlighting the influence of surface morphology on electrocatalytic performance.

Graduate Research Assistant, University at Buffalo, SUNY   Aug 2015 – May 2020
Dissertation: Multiscale Modeling of Charge Dynamics in Photoelectrocatalytic Systems
- **Developed PyCD**, a scientific software for multi-scale, multi-physics kinetic Monte Carlo simulations, enabling prediction of solar energy conversion in crystalline photoelectrodes.
- **Characterized charge transport behavior** using *first-principles* atomistic modeling in various $BiVO_4$-based photoelectrode materials, providing fundamental insights for rational design.
- **Developed a mechanistic model** for enhanced carrier mobility in S-doped $BiVO_4$, recommending facet engineering guidelines for improved electrochemical performance.

Graduate Research Assistant, Indian Institute of Technology, Guwahati   July 2012 – May 2014
Thesis: Self-propelling micro-swimmers for continuous hydrogen production
- **Designed self-propelling** FeNP-coated polymer micromotors for rapid on-site hydrogen generation.
- **Characterized microstructure** of FeNPs using FESEM and TEM, chemical composition with EDX, XRD, FTIR, and Raman, and functional properties via VSM and GC.
- **Powered a portable PEM fuel cell** using ferrobots, providing continuous H_2 supply from formic acid decomposition and O_2 from catalytic decomposition of hydrogen peroxide.

Senior Thesis, National Institute of Technology, Calicut, India   Jul 2011 – Apr 2012
Project: Modeling and Simulation of Three-Way Catalytic Converters
- **Modeled complex interactions** in a three-way catalytic converter, describing two-dimensional gaseous flow coupled with surface catalytic reactions, and mass and heat transfer processes.
- **Characterized transient behavior** of a monolithic single channel using numerical simulations with FEM and solved systems of partial and ordinary differential equations in MATLAB.

TECHNICAL SKILLS
- *Computational Chemistry* **|** VASP, Quantum Espresso, CP2K, Gaussian, NAMD, VMD, VESTA, Blender, Turbomole
- *Programming & Scripting Languages* **|** Python (NumPy, SciPy, Pandas), MATLAB, Mathematica, Maple, Tcl/Tk, Scilab, BASH, VBA
- *Software Development* **|** Git, GitHub, GitHub Actions, Travis CI, Codecov, Visual Studio Code
- *Data Science, ML, AI* **|** scikit-learn, PyTorch, TensorFlow, NumPy, SciPy, Pandas, Matplotlib
- *High-Performance Computing* **|** Experience with running large-scale serial/parallel calculations of electronic structure and atomistic simulations on high-performance computing (HPC) systems.
- *Automation* **|** Highly automated and optimized work-flow with Linux command-line tools and scripting.