Sudheesh Kumar Ethirajan

Ph.D. student in Chemical Engineering · University of California, Davis
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Education

University of California Ph.D. in Chemical Engineering; Prof. Ambarish Kulkarni — *Davis, CA (10/2021 - present)*
Carnegie Mellon University M.S. in Chemical Engineering; Prof. Zachary Ulissi — *Pittsburgh, PA (09/2019 - 12/2020)*
Indian Institute of Technology B.Tech. in Chemical Engineering (Honors); Minor in CSE — *Dhanbad, India (07/2014 - 07/2018)*

Research Interests

Computational Catalysis, Molecular Simulations, Accelerated Materials Discovery, Rare-events Sampling, Machine Learning

Projects & Research Experience

University of California — *Davis, CA*

Deep Potentials for studying adsorption & diffusion processes in Metal-Organic Frameworks — *(05/2022 – present)*

- Bench-marked various XC functionals with lattice length and bulk modulus of ZIF-8.
- Performed sequential relaxations and ab-initio molecular dynamics simulations for different ZIF-8 functionalizations.
- Identified transition states through Nudged Elastic Band calculations for linker diffusion through MOF pores.
- Sampled high-energy states (rare events) through constrained molecular dynamics of linkers at MOF pores.
- Constructed Deep Neural Network potentials using Deep-MD package.

Self consistent DFT-Microkinetic models for surface catalyzed reactions — *(07/2021 – present)*

- Generated automatic reaction mechanisms for partial oxidation of CH4 on Pt catalyst.
- Developed a python module for generating an Adjacency list graph representation for any molecule or surface-adsorbed species.
- Extracted thermodynamic quantities and constructed NASA polynomials from DFT calculated values for surface reactions.
- Designed a workflow integrating ASE-VASP-RMG python packages to generate automated reaction mechanisms.

Carnegie Mellon University — *Pittsburgh, PA*

Molecular simulations of Nafion ionomer/ Pt interfaces — *(01/2020 – 12/2020)*

- Studied the phenomena of O2 diffusion in fuel cell.
- Performed plane-wave DFT calculations (VASP) to model Nafion – Pt (111) interactions.
- Accelerated DFT calculations with Amptorch – a ML Python package.

Publications

- Price, T., Rana, R., **Ethirajan, S. K.**, Holton, S. J. & Kulkarni, A. R. An Introductory Primer for Modeling Atomically Dispersed Catalysts using Density Functional Theory. *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*, (2022).
- Sengupta, A., **Ethirajan, S. K.**, Kamaz, M., Jebur, M. & Wickramasinghe, R. Synthesis and characterization of antibacterial poly ionic liquid membranes with tunable performance. *Sep Purif Technol* 212, 307–315 (2019).
- **Ethirajan, S. K.** *et al*. Single-Step Synthesis of Novel Polyionic Liquids Having Antibacterial Activity and Showing π-Electron Mediated Selectivity in Separation of Aromatics. *Chem* 3, 4959–4968 (2018).

Conference Presentations

- Tiwari, N., **Ethirajan, S. K.** & Ulissi, Z. All-Atom Molecular Dynamics Study for O2 Permeation in a Nafion Polyelectrolyte Membrane. *AIChE 2020 annual conference (virtual)*, San Francisco, USA.
- Sengupta, A., **Ethirajan, S. K.**, Jebur, M., Kamaz, M. & Wickramasinghe, S. R. Imidazolium Based Poly (ionic liquids), the Tunable Membranes Having Antimicrobial Activity. *AIChE 2018 annual conference*, Pittsburgh, USA.

Technical Skills

Programming	Python, R, Bash, MATLAB
Python packages	NumPy, SciPy, Pandas, Scikit-Learn, TensorFlow, ASE, RDKit, RMG, Jupyter, Seaborn, Plotly, Matplotlib
Modeling & Simulation	VASP, QE, LAMMPS, GAMS, COMSOL
Software tools	Git, GitHub, LaTeX