Hunter Pauker

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Summary

- Four+ years of research experience in computational chemistry and catalysis
- Technical expertise in *ab initio* electronic structure simulations, DFT and CCSD(T)
- Employed and refined machine learning methods to accelerate and optimize materials design
- Developed programs in MATLAB, Python, and Bash to streamline workflows for computational chemistry software, and predict and interpret data of catalytic systems.
- Experience in LINUX/High Performance Computing environments
- Created robust micro-kinetic models of complex reaction networks of catalytic behavior
- Presented research findings at National Conference and published peer reviewed papers
- Educated undergraduate students in computational chemistry, catalysis, LINUX environments/High Performance Computing, MATLAB, data analysis, and multivariate regressions
- Experience in various ML techniques: Principal Component Analysis/Regression, Partial Least Squares Regression, Lasso/Ridge/Elastic Net, Support Vector Machines
- Strong understanding of the key chemical engineering principles: thermodynamics, transport phenomena, chemical kinetics, and reactor engineering

Education

University of California, Irvine

Ph.D. in Chemical Engineering 2019–2024
Thesis: Data Directed Optimization of Catalysts
Advisor: Robert Nielsen

- Utilized tools of computational chemistry and machine learning to study the structure-to-function relationships in families of catalysts
- Applied first-principles simulations to interpret experimental observations and guide lab results
- Used combined DFT and CCSD(T) simulation to map Free Energy Surfaces (FES) of catalytic cycle of the electrocatalytic reduction of CO_2 to formate with cyclopentadienyl complexes of first-row transition metals
- Used ML techniques to analyze said FES to reveal degrees of freedom for catalyst optimization and maximum performance within the composition space
- Studied methane oxidation with Ir^{III} complexes and ligands that varied in their simga bonding, pi backbonding, steric properties, and charge
- Utilized various regression models to relate these chemical properties to DFT-derived FESs and predicted the FESs of novel Ir^{III} catalysts (i.e. designed)
- Iteratively refined and trained models of all previously mentioned systems, towards optimum catalyst performance

M.S. in Chemical Engineering 2019–2021
Coursework and research in computational chemistry and data-driven catalyst discovery

University of California, Davis

B.S. in Chemical Engineering 2014–2019
Ceramics Instructor at UC Davis Craft Center 2016–2019
Pedagogical Research, Advisor: Professor William Ristenpart 2017–2019

- Designed experiments to teach principles of chemical engineering through beer brewing

Research Interests

Computational chemistry, data-driven catalyst discovery, machine learning for scientific discovery, reproducible modeling workflows, accessible science, interdisciplinary intersections of art and science.

Conference Presentations

ACS Fall 2023, Computers in Chemistry Division
Session: Data Science for Catalysis: Automated Synthesis, Process Optimization, and Catalyst Discovery
Data-Directed Optimization of Catalysts

Teaching Experience

UC Irvine
Undergraduate Mentor 2020–2023

- Educated students in the basics of electronic structure simulations, and tools necessary to perform these calculations: LINUX environments, high performance computing, Bash, and Vim
- Facilitated discussions with students to integrate and link material from their coursework with principals of chemical engineering, catalysis, and electronic structure calculations
- Introduced students to multivariate regression techniques, and data analysis in MATLAB

UC Davis Craft Center
Instructor, Ceramics Program 2016–2019

- Designed and executed lesson plans to teach the basics of making pottery on the wheel: throwing, drying, trimming, and glazing
- Designed and executed lesson plans to teach advanced wheel throwing for making wide vessels (bowls, plates, and platters)
- Supported students individually and in groups to address learning needs and promote equitable progress among the class

Technical Skills

Computational Chemistry: ORCA, TURBOMOLE, Molden
Programming Languages: Python, MATLAB, Bash, HTML/CSS
Machine Learning: PCA, PLSR, LASSO, Ridge, SVM

Artistic Practice & Fabrication

Ceramics: Wheel throwing, trimming, wedging, large-scale hand building
Formulation: Glaze and clay body design, slip casting, mold making
Digital Fabrication: CAD design, SLA resin 3D printing
Other Media: Drawing, painting, fiberglass resin layup

References

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