PARTHO KUMAR PAUL

Ph.D. Candidate, Organic Chemistry — University of California, Irvine
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PROFESSIONAL SUMMARY

Physical organic chemist with expertise bridging experimental mechanistic study and computational modeling, completing a Ph.D. focused on the design and characterization of redox-active molecules for electrochemical CO_2 capture and other energy storage related applications. Currently a DOE SCGSR Fellow at Brookhaven National Laboratory conducting pulse radiolysis experiments to probe ultrafast electron transfer and radical formation mechanisms of biologically relevant redox-active compounds. This work is directly relevant to understanding catalytic intermediates in small molecule activation. I have also been trained in transition-metal-mediated transformation of olefins (cobalt-catalyzed radical–polar crossover reactions) with experience correlating molecular structure to reactivity. Incoming visiting researcher at RIKEN, where TDDFT simulation of reduced intermediates on the Fugaku supercomputer will deepen my proficiency in density functional theory applied to molecular systems. I have built Python,jss, and html-based data analysis and automation, with growing capabilities in machine learning for predictive modeling of chemical reactivity.

EDUCATION

Ph.D., Organic Chemistry *Expected Summer 2026*
University of California, Irvine | Advisor: Prof. Jenny Y. Yang

- Dissertation: Design, synthesis, and electrochemical characterization of bio-inspired redox-active molecules for CO_2 capture in organic and aqueous media
- Eugene Cota-Robles Fellowship (1st & 4th Year) | Dissertation Year Fellowship (Summer 2025)

B.S., Chemical Engineering (Nanotechnology Emphasis), Minor: Chemistry *2020*
University of California, Riverside

- UC LEADS Scholar (2018), Bourns Scholar, Research mini-grant recipient

RESEARCH EXPERIENCE

Visiting Researcher (Incoming) — Computational Chemistry *Jun 2026 – Aug 2026*
RIKEN Center for Computational Science, Kobe, Japan

- Selected for DOE SCGSR International Research Collaboration Award (IRCA) to perform TDDFT computational chemistry on the Fugaku supercomputer, modeling excited-state properties and electronic structure of molecular systems.
- Will be applying density functional theory (DFT) methods to characterize reduced organic intermediates via spectral simulation and energy-minimized structure and pka calculation.
- Developing Python-based workflows for high-performance computing job management, data extraction, and ML-assisted analysis of computational results.

DOE SCGSR Fellow / Visiting Research Scientist *Jan 2026 – Jun 2026*
Brookhaven National Laboratory, Chemistry Division, Upton, NY

- Designing and executing pulse radiolysis experiments to probe ultrafast electron transfer kinetics and radical formation mechanisms in water-soluble flavin derivatives. This led to generation of quantitative rate constants and transient absorption spectra relevant to understanding catalytic intermediates.
- Analyzing time-resolved spectroscopic datasets to extract mechanistic insights into one-electron redox processes, structure–reactivity relationships, and the fate of reactive intermediates in solution.
- Collaborating directly with senior BNL scientists in the Artificial Photosynthesis group and across Chemistry Division, integrating experimental results with computational and mechanistic models.
- Familiar with BNL's research infrastructure, collaborative culture, safety protocols, and DOE-funded multi-institutional center operations.

Graduate Student Researcher — Electrochemical CO_2 Capture *Apr 2024 – Present*
Yang Lab, University of California, Irvine

- Designed, synthesized, and characterized 10+ novel redox-active organic molecules (hydroxymethylated quinones, alloxazine/flavin derivatives) for electrochemical CO_2 capture, systematically correlating molecular structure with redox potentials, electron transfer kinetics, and stability.

- Performed cyclic voltammetry, bulk electrolysis, and spectroelectrochemistry to quantify binding thermodynamics and identify relevant operable pathways—skills directly transferable to evaluating molecular catalysts for CO_2 reduction.
- Investigated degradation mechanisms and transformation pathways using multi-technique characterization (NMR, UV-Vis, FTIR, GC-MS, LC-MS, ESI-MS), building expertise in tracking reactive intermediates and catalyst deactivation.
- Built Python-based data analysis and automation software for electrochemical and spectroscopic workflows, improving reproducibility and enabling systematic structure–property analysis across compound libraries.

Graduate Student Researcher — Transition-Metal Catalysis *Aug 2021 – Mar 2024*
Pronin Lab, University of California, Irvine

- Investigated cobalt-catalyzed radical–polar crossover reactions involving metal-hydride hydrogen atom transfer (MHAT)—homogeneous transition-metal catalysis directly relevant to cascade and tandem catalytic strategies for small molecule activation.
- Systematically optimized catalyst structure, ligand environment, reagent stoichiometry, and reaction conditions to control selectivity and yield in multiple alkene functionalization reaction.
- Performed ^{18}O isotopic labeling studies and detailed product characterization (NMR,MS) to elucidate mechanistic pathways, including the roles of radical and polar intermediates in catalytic cycles.
- Executed air-sensitive synthesis (Schlenk line, glovebox) of transition-metal complexes and organic substrates, developing practical expertise in handling catalytically active metal species.

TECHNICAL SKILLS

Computational: TDDFT (Fugaku supercomputer), density functional theory, electronic structure calculations, Python scripting for HPC workflows and data analysis

Programming & Data Science: Python (NumPy, SciPy, Matplotlib, pandas), data automation and visualization pipelines, building proficiency in TensorFlow/PyTorch for predictive modeling of chemical reactivity

Experimental Techniques: Pulse radiolysis, cyclic voltammetry, bulk electrolysis, spectroelectrochemistry, transient absorption spectroscopy, NMR, UV-Vis, IR/FTIR, GC-MS, LC-MS, ESI-MS

Synthesis & Catalysis: Organic synthesis, transition-metal catalysis, air-sensitive techniques (Schlenk line, glovebox), isotopic labeling (^{18}O), molecular design and reaction optimization

Software: Origin, ChemDraw, MestReNova, Git, Linux/Unix, Microsoft Office Suite, Igor Pro

PUBLICATIONS

Paul, P. K.; Lin, C. C.; Yang, J. Y. *Design, Synthesis, and Studies of Hydroxymethylated Quinone Derivatives for Electrochemical CO_2 Capture.* Manuscript in preparation.

Paul, P. K.; Yang, J. Y. *Synthesis and Evaluation of Charged Flavin Derivatives for pH-Swing Mediated CO_2 Capture.* In preparation.

COMMUNICATION & MENTORING

Teaching Assistant & BLOOM Faculty Intern *Aug 2021 – Present*
UC Irvine & Irvine Valley College

- Led discussion sections, labs, and independently delivered lectures for 4+ years across general and organic chemistry; maintained a private tutoring practice for 8+ years.
- Mentored 3+ undergraduate researchers on synthesis, characterization techniques, and instrument operation; experienced in onboarding collaborators in multi-institutional research settings.
- Elected Representative (AGS) for the School of Physical Sciences, coordinating across faculty, administration, and student body.

AWARDS & FELLOWSHIPS

- DOE Office of Science Graduate Student Research (SCGSR) Fellowship — Brookhaven National Laboratory (2026)
- DOE SCGSR International Research Collaboration Award (IRCA) — RIKEN, Japan (2026)
- Eugene Cota-Robles Fellowship — UC Irvine (1st & 4th Year)
- School of Physical Sciences Dissertation Year Fellowship — UC Irvine (Summer 2025)
- UC LEADS Scholar — UC Riverside (2018)