PARTHO KUMAR PAUL

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

Physical scientist with an interdisciplinary trajectory spanning organic synthesis, electrochemistry, ultrafast spectroscopy, and high-performance computation. My research career reflects a deliberate arc of intellectual growth: from mastering multi-step air-sensitive synthesis and transition-metal catalysis, to designing and characterizing novel redox-active molecules for electrochemical CO_2 capture, to probing ultrafast electron transfer mechanisms via pulse radiolysis, and now extending into TDDFT computational chemistry on the Fugaku supercomputer. At each stage I have sought out unfamiliar domains, demonstrating the adaptability and curiosity that LLNL's Design Physics Division values. I bring a rare experimental–computational versatility: comfort with Schlenk lines and gloveboxes alongside proficiency in Python-driven data pipelines and density functional theory. I am eager to apply this breadth—and deepen it—across any of the Division's research areas, from chemical physics and radiation transport to computational modeling and diagnostic development.

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 — 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 electronic structure of molecular systems.
- Applying density functional theory methods to characterize reduced organic intermediates via spectral simulation and energy-minimized geometry and pKa calculations.
- Developing Python-based workflows for high-performance computing job management, automated data extraction, and ML-assisted analysis of computational results across large compound libraries.

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, generating quantitative rate constants and transient absorption spectra for reactive intermediates.
- Analyzing time-resolved spectroscopic datasets to extract mechanistic insights into one-electron redox processes, structure–reactivity relationships, and the fate of short-lived radicals in solution.
- Collaborating across BNL's Chemistry Division with senior scientists in the Artificial Photosynthesis group, integrating experimental pulse radiolysis results with computational and mechanistic models.

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, map operative pH-swing pathways, and identify degradation mechanisms—skills transferable to any energy-relevant molecular characterization.

- Investigated 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 across timescales.
- Built Python-based data analysis and automation pipelines for electrochemical and spectroscopic workflows, 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), developing detailed mechanistic understanding of selectivity in olefin functionalization.
- Systematically optimized catalyst structure, ligand environment, and reaction conditions to control selectivity and yield, building transferable skills in experimental design and parameter optimization.
- Performed ^{18}O isotopic labeling studies and multi-technique product characterization (NMR, MS) to elucidate radical and polar intermediates in catalytic cycles.
- Executed air-sensitive synthesis (Schlenk line, glovebox) of transition-metal complexes, developing rigorous handling skills for reactive and unstable species.

TECHNICAL SKILLS

Computational: TDDFT (Fugaku supercomputer), density functional theory, electronic structure calculations, Python scripting for HPC workflows and data analysis, building proficiency in ML/TensorFlow for predictive modeling
Programming & Data: Python (NumPy, SciPy, Matplotlib, pandas), JavaScript/HTML data tools, Git, Linux/Unix, automated data pipelines for electrochemical and spectroscopic analysis
Experimental: Pulse radiolysis, transient absorption spectroscopy, cyclic voltammetry, bulk electrolysis, spectroelectrochemistry, NMR, UV-Vis, IR/FTIR, GC-MS, LC-MS, ESI-MS
Synthesis & Characterization: Multi-step organic synthesis, transition-metal catalysis, air-sensitive techniques (Schlenk line, glovebox), isotopic labeling (^{18}O), molecular design and reaction optimization
Software: Origin, ChemDraw, MestReNova, Igor Pro, Microsoft Office Suite

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)