John Cokas

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Education

Yale University — New Haven, CT
Graduate Student, PhD Program — August 2025 – Present

- Coursework:

Molecules and Radiation I & II	Introduction to Quantum Computing	Introduction to Machine Learning
Statistical Mechanics I & II	Advanced Quantum Mechanics	

University of California, Los Angeles — Los Angeles, CA
Bachelor of Science in Chemistry — June 2024

- GPA: 3.91/4.00
- Awards: Dean's List and Arthur Furst Commencement Award
- Relevant coursework:

Quantum Chemistry	Thermodynamics	Topics in Physical Chemistry
Materials Chemistry Lab	Physical Chemistry Lab	Advanced Inorganic Chemistry

Relevant Experience

Yale University — New Haven, CT
Research Assistant — February 2025 – Present

- Simulated quantum dynamics of 11-cis-retinal in rhodopsin classically and on a simulated quantum circuit.
- Coded simulation to machine learn pulses of lights to produce desired changes in vibrational modes.

UCLA Department of Chemistry and Biochemistry — Los Angeles, CA
Undergraduate/Staff Researcher — April 2023 – September 2024

- Calculated self-proposed dehydrogenation mechanisms for a novel dehydrogenation catalyst using DFT.
- Performed DFT calculations using VASP of clusters sintering on an alumina surface and analyzed results.
- Sampled isobutene binding modes on a platinum/germanium cluster supported by alumina.
- Collaborated with researchers at the University of Hawaii and University of Utah.

Community/Volunteer Experience

Alpha Chi Sigma, Beta Gamma Chapter — Los Angeles, CA
Member — April 2023 – Present

- Tutored chemistry and physics students in upper and lower division courses.
- Actively engaged in all fraternal events and helped set up various fraternal events.

Skills

- I am proficient with Orca, VASP, ASE, and Spartan which are all chemical modeling/calculation programs.
- Bash scripting and Python
- Proficient in Microsoft Word, PowerPoint, Excel, Adobe Photoshop, HitFilm Express, and their analogs.

Publications

1) Biswas, S.**, Cokas, J.**, Gee, W. *et al.* Unconventional low temperature decomposition of a saturated hydrocarbon over atomically-dispersed titanium-aluminum-boron catalyst. *Nat Commun* **16**, 6793 (2025). https://doi.org/10.1038/s41467-025-62112-2
   ** These Authors contributed equally.