KYOGO NAGASHIMA

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EDUCATION

California Institute of Technology — Pasadena, California
PhD in Chemistry — Starting Fall 2024

Oberlin College — Oberlin, Ohio
High Honors in Chemistry, Minor in Computer Science — Spring 2024
GPA: 3.99/4.33

Hokkaido International School — Hokkaido, Japan
GPA: 3.96/4.00 — Spring 2020

PUBLICATIONS

Liu, D.‡, **Nagashima, K.‡**, Liang, H., Yue, X., Chu, Y., Chen, S., Ma, J. Arene Reduction by Energy Transfer Catalysis Enabled Hydrogen Atom Transfer: Advancing the Chemoselectivity. *Angew. Chem., Int. Ed*, 2023. DOI: 10.1002/anie.202312203 (recently accepted).

Buck, L.D. ‡, Paladino, M.M. ‡, **Nagashima, K**., Holtzman, J.S., Brezel, E.R., Urso, S.J., Ryno, L.M. Temperature-dependent influence of FliA overexpression on PHL628 E. coli biofilm growth and composition. *Frontiers in Cellular and Infection Microbiology*, 2021, 11, 775270. DOI: 10.3389/fcimb.2021.775270

‡: equal contribution

ORAL PRESENTATIONS

"Investigating the Excited State Properties of CBI-Serotonin using TD-DFT", *Oberlin College Honors Talk*, Oberlin College, Oberlin, Ohio, May 5th, 2024.

"Investigating the Fluorescence Quenching of CBI-Serotonin using TD-DFT and Fluorescence Spectroscopy", *Oberlin College Honors Proposal*, Oberlin College, Oberlin, Ohio, November 29th, 2023.

"Modifying the Oxidation State of a Bis(amido)bis(phosphine) Iron (II) complex", *Ohio5 Research Symposium*, The Ohio State University, Columbus, Ohio, July 26th, 2023.

"Influence of Sugars on Biofilm Formation and Composition in E. coli", *Oberlin College Undergraduate Research Symposium*, Oberlin College, Oberlin, Ohio, May 13th, 2022.

POSTER PRESENTATIONS

"Modifying the Oxidation State of a Bis(amido)bis(phosphine) Iron (II) complex", *Ohio Inorganic Weekend*, Bowling Green State University, Bowling Green, Ohio, November 17th, 2023 (*An updated version of the poster prepared for the Ohio5 Research Symposium*).

"Modifying the Oxidation State of a Bis(amido)bis(phosphine) Iron (II) complex", *Ohio5 Research Symposium*, The Ohio State University, Columbus, Ohio, July 26th, 2023.

"Computational Investigation of Energy Landscapes and Agostic Interactions in Metal-Assisted C-H Cleavage", *Oberlin College Undergraduate Research Symposium*, Oberlin College, Oberlin, Ohio, April 28th, 2023.

"Influence of Sugars on Biofilm Formation and Composition in E. coli", *ACS National Spring 2023 Meeting*, Indianapolis, Indiana, March 28th, 2023.

SELECTED RESEARCH PROJECTS

Using Machine Learning to Predict Heterogeneous Catalyst Performance Spring 2024
Advisor: Prof. Adam Eck, Oberlin College Computer Science Department

- Used various machine learning models such as neural networks, random forests, and support vector machines to predict heterogeneous catalyst performance.
- GitHub Link: https://github.com/KyogoNagashima/CatalystDatabaseProject

Investigating the Fluorescence Quenching of CBI-Serotonin (Honors Thesis) Fall 2023 to Spring 2024
Advisor: Prof. Rachel Saylor, Oberlin College Chemistry/Biochemistry Department
Consultant: Prof. Shane Parker, Case Western Reserve University Chemistry Department

- Investigated the mechanisms of fluorescence quenching of a strongly fluorescent cyanobenz[f]isoindole product when serotonin is the primary amine in the molecule.
- Used fluorescence spectroscopy and time-dependent density-functional-theory (TD-DFT) to elucidate fluorescence quenching mechanisms.

Modifying the Oxidation State of a Bis(amido)bis(phosphine) Iron(II) Catalyst Summer 2023
Advisor: Prof. Christine Thomas, The Ohio State University Chemistry/Biochemistry Department

- Conducted organic/inorganic synthesis of a bis(amido)bis(phosphine) iron(II) catalyst.
- Successfully isolated crystal structure of the catalyst with an oxidized iron center.
- Used various characterization techniques such as NMR, paramagnetic NMR, IR, X-ray crystallography.

Computational Study of Hydrogen Atom Transfer by Energy Transfer Catalysis Fall 2022 to Spring 2023
Advisor: Prof. Shuming Chen, Oberlin College Chemistry/Biochemistry Department

- Computationally modelled reduction of quinolines through hydrogen atom transfer enabled by energy transfer catalysis using density functional theory (DFT) calculations.
- Conducted computational calculations to support hypothesis that triplet energies accounts for the origins of selectivity rather than reduction potentials.
- This work was published in *Angewandte Chemie*.

Computational Study of Agostic Interactions in Metal Assisted C-H Cleavage Fall 2022 to Spring 2023
Advisor: Prof. Shuming Chen, Oberlin College Chemistry/Biochemistry Department

- Studied metal-assisted C-H activation reactions involving significant agostic interactions with DFT calculations by investigating the effects of various ligands on the energy landscape.
- Conducted analysis of mechanism with original Python/Java based scripts.

Thioketone Preference over Ketone Directing Groups in C-H Arylation Fall 2022 to Spring 2023
Advisor: Prof. Shuming Chen, Oberlin College Chemistry/Biochemistry Department

- Investigated the origins of thioketone preference over ketone directing groups in C-H activation through Pd(II) catalyzed arylation reactions through DFT calculations.
- Calculated reactions barriers with added tether groups to investigate effects on structural geometries to investigate the origins of thioketone preference over ketone directing groups.

Effects of Environmental Sugars on Biofilm Formation Fall 2021 to Spring 2022
Advisor: Prof. Lisa Ryno, Oberlin College Chemistry/Biochemistry Department

- Explored the effects of various pentose sugars on the effects of biofilm formation in *E. coli* bacteria.
- Designed a workflow for the lab to systematically investigate other understudied sugars.
- Produced preliminary results used in a recently funded NSF grant (MCB-2226953) of $534002.

Effects of the *yhjH* Gene on Biofilm Formation Summer 2021
Advisor: Prof. Lisa Ryno, Oberlin College Chemistry/Biochemistry Department

- Studied the effects of the yhjH gene on biofilm formation in *E. coli* bacteria.
- Used a variety of techniques in molecular biology and biochemistry including qPCR and crystal violet assay to assess both genomic and phenotypic effects of overexpression of the yhjH gene through the effects of internal c-di-GMP levels.

RESEARCH SKILLS

Computational Chemistry:

- Elucidating reaction mechanisms of organometallic and organic reactions using DFT.
- TD-DFT techniques for photochemical applications and charge-transfer reactions.
- Molecular orbital and natural transition orbital (NTO) analysis.
- Conformer search using meta-dynamical simulations (*Conformer-Rotamer Ensemble Sampling Tool*).
- Analysis of atomic charges, bond lengths, and bond angles through original Java/Python scripts.

Programming:

- Machine Learning based project to predict heterogeneous catalyst performance.
- Proficient in Python, Java, and C, with basic understanding of data structures, algorithms, and systems.
- Developed Python and Java programs for data analysis to use in computational chemistry research.
- Experience of data analysis and statistical modelling using R.

Synthetic Inorganic Chemistry:

- Organic/inorganic synthesis of transition metal-based catalyst.
- Air sensitive chemistry using Schlenk lines and glove box.
- Characterization using paramagnetic NMR, NMR, and FTIR spectroscopy.
- Growing crystal structures of metal complexes for characterization by X-ray crystallography.

Biochemistry:

- Basic Microbiology and Cell Culturing techniques using *E. coli*.
- Extensive use of qPCR, gel-electrophoresis, and western blotting.
- Proficient use of confocal laser scanning microscope (CLSM).

RELATED JOB EXPERIENCES

Teaching Assistant for General Chemistry, Oberlin College Spring 2024

- Helped facilitate an introductory chemistry course of about 30 students.
- Held two interactive review sessions every week outside of class with self-prepared worksheets.
- 42 hours of session leading with higher average scores recorded for students attending help sessions.
- Recorded highest attendance with an average of 10 students attending per week.

Tutor for General Chemistry II, Oberlin College Spring 2024

- Helped 4~5 students every week on concepts such as thermodynamics, equilibrium, and kinetics.
- Approximately 60 hours of tutoring for a total of 6 students.

Grader for Quantum Chemistry, Oberlin College Spring 2024

- Grading problem sets, providing feedback to students for an upper-level quantum chemistry class.

Tutor for General Chemistry I, Oberlin College Fall 2023

- Helped 2~3 students every week on concepts such as quantum chemistry, basic reactions, and bonding.
- Approximately 30 hours of tutoring for a total of 3 students.

Tutor for Introductory Physics, Oberlin College Fall 2022

- Helped 4~5 students every week, explaining concepts slowly from the basics to build up for applications to complex problems.
- 38 hours total of tutoring.

Teaching Assistant for Introductory Biology, Oberlin College Fall 2021

- Helped facilitate an introductory biology course of about 30 students.
- Held two interactive review sessions every week outside of class with self-prepared worksheets.
- 42 hours of session leading.

HONORS AND AWARDS

Harry N. Holmes Prize 2024
Award by Oberlin College Department of Chemistry & Biochemistry

William B. and Hellen K. Miller Memorial Scholarship 2023
Award by Oberlin College Department of Chemistry & Biochemistry

Frank Fanning Jewett Award 2022
Award by Oberlin College Department of Chemistry & Biochemistry

Oberlin Undergraduate Research Featured Researcher 2021
Awarded by Oberlin Office of Undergraduate Research

Edwin O. Reischauer Scholarship 2020 to 2024
Awarded by Oberlin College of Arts and Science

RELEVANT COURSEWORK

Chemistry and Physics: Chemical & Statistical Thermodynamics, Quantum Chemistry and Kinetics, Inorganic Chemistry, Synthesis Laboratory, Organic Mechanism and Synthesis, Organic Chemistry, Analytical Chemistry, Structure & Reactivity (GenChem I), Chemistry Principles (GenChem II), Mechanics and Relativity (Physics I), Elect/Magnetism/Thermo (Physics II)

Computer Science: Machine Learning, Algorithms, Data Structures, Systems Programming, Intro to CS.

Math: Linear Algebra, Statistics and Modelling, Discrete Math, Multivariable Calculus

Other Self-studied Topics: Classical Mechanics, Statistical Mechanics, Theories of Computational Chemistry

OTHER SKILLS

Language: Native level in both English and Japanese in speaking, reading, and writing.

Music: Piano (7 years), Cello (10 years).

Hobbies: Soccer, Futsal, Hiking, Camping, Gardening.

REFERENCES

Dr. Christine Thomas (Research Mentor)
Chemistry/Biochemistry Department
The Ohio State University
Email: thomas.3877@osu.edu

Dr. Lisa Ryno (Research Mentor)
Chemistry/Biochemistry Department
Oberlin College
Email: lryno@oberlin.edu

Dr. Rachel Saylor (Research Mentor)
Chemistry/Biochemistry Department
Oberlin College
Email: rsaylor@oberlin.edu

Dr. Shane Parker (Research Consultant)
Chemistry Department
Case Western Reserve University
Email: shane.parker@case.edu

Dr. Shuming Chen (Research Mentor)
Chemistry/Biochemistry Department
Oberlin College