Heejune Park **Last update: Feb. 20th, 2023**

CONTACT INFORMATION
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EDUCATION

University of California, Davis 2019–Present

- Ph.D. in Department of Chemistry (Computational Chemistry), GPA: 3.84/4.00
- Advisor: Prof. Lee-Ping Wang

University of San Francisco 2017–2019

- M.S. in Department of Chemistry (Physical Chemistry), GPA: 4.00/4.00
- Advisor: Prof. Giovanni Meloni
- Thesis: *Synchrotron Photoionization Study of 2,5-Dimethylfuran Oxidation Initiated by $O(^3P)$ Atoms, and Computational Studies of Superalkali Species: Li_3F_2*

California State University, Chico 2012–2016

- B.S. in Department of Chemistry & Biochemistry (Physics Minor), GPA: 3.35/4.00
- Advisor: Prof. Randy Miller

RESEARCH EXPERIENCE

Developing software tools for exploring potential energy surfaces 2020-Present
University of California, Davis

- Developing a workflow that can refine molecular dynamics simulation trajectories in an automated manner. The workflow can distribute quantum calculations to multiple computing nodes and store results based on a database platform.

Oxidation reaction pathways of biofuel molecules 2017–2019
Lawrence Berkeley National Laboratory & University of San Francisco

- Employed synchrotron radiation to photoionize products/intermediates of biofuel oxidation reactions initiated by various radicals. The ionized species were detected through TOF-MS. Computational methods were utilized to probe the reaction pathways.

Computational studies of superatom species 2017–2019
University of San Francisco

- Theoretical studies of superatom molecules that have strong tendency of either accepting or donating an electron to other species.

PUBLICATIONS

1. Giustini, A.; Aschi, M.; **Park, H.**; Meloni, G. **2021**, "Theoretical and experimental study on the $O(^3P)$ + 2,5-dimethylfuran reaction in gas phase". *PCCP*, 23 (35), 19424-19434.

2. Giovanni, M.; Giustini, A.; **Park, H**. **2021**, "CO_2 activation within a superalkali-doped fullerene". *Front. Chem*, 9 , 712960.

3. Price, C.; Winfough, M.; **Park, H.**; Meloni, G. **2018**, "Computational investigation of LiF containing hypersalts". *Dalton Transactions*, 47 (37), 13204-13213.

4. **Park, H.**; Meloni, G. **2018**, "Capturing volatile organic compounds employing superalkali species". *ChemPhysChem*, 19 (17), 2266-2271.

5. **Park, H.**; Meloni, G. **2018**, "Activation of dinitrogen with a superalkali species, Li_3F_2". *ChemPhysChem*, 19 (3), 2266-2271. *Featured on Journal Cover*

6. **Park, H.**; Meloni, G. **2017**, "Reduction of carbon dioxide with a superalkali". *Dalton Transactions*, 46 (35), 11942-11949.

Poster Presentations

1. **Park, H.**; Meloni, G. "Investigation of 2,5-dimethylfuran oxidation reaction initiated by $O(^3P)$ atoms *via* synchrotron photoionization."
Division of Physical Chemistry Poster Session: **257th ACS National Meeting**, Orlando. April 2019

2. **Park, H.**; Meloni, G. "Reduction of CO_2 and N_2 using the Li_3F_2 superalkali."
Division of Physical Chemistry Poster Session: **255th ACS National Meeting**, New Orleans. March 2018

Teaching Experience

TA for Quantum Chemistry (Graduate Course) — Winter 2023
University of California, Davis

TA for Physical Chemistry — Summer 2022
University of California, Davis

TA for Statistical Thermodynamics (Graduate Course) — Fall 2020; Fall 2022
University of California, Davis

Head TA for General Chemistry — Spring 2020
University of California, Davis

TA for General Chemistry — Winter 2020
University of California, Davis

TA for Honors General Chemistry — Fall 2019
University of California, Davis

TA for General and Analytical Chemistry — 2017-2019
University of San Francisco

Honors and Awards

- 2021 MolSSI Software Seed Fellowship — 2021
The Molecular Sciences Software Institute
- American Institute of Chemists' Foundation Award — 2019
University of San Francisco
- Graduate Award of Achievement in Teaching — 2019
University of San Francisco
- Ron Najafi Emery Pharma Service Innovation Award — 2018
University of San Francisco
- Chemistry Research Award — 2018
University of San Francisco

Professional Affiliations

- American Chemical Society — 2015–Present
Graduate student member
- Student Affiliates of the American Chemical Society — 2015–2016
Student member at California State University, Chico

Other Skills

- Programming Language: Python, SQL
- Operating System: Linux, Windows
- Quantum Chemistry Software: geomeTRIC, TeraChem, QChem, Psi4, Gaussian
- Languages: Korean (Native), English (Fluent), Japanese (Intermediate), and Chinese (elementary)