# Julius J. Oppenheim

505 Beacon St Apt 6, Boston, MA 02215 • joppenhe@mit.edu • (845) 269-9905

#### Education

Massachusetts Institute of Technology Ph.D. in Chemistry, expected May 2024 Cambridge, MA GPA: 5.0/5.0

Research Advisor: Professor Mircea Dincă

Dissertation: Tailoring Metal-Organic Frameworks for Water Harvesting

California Institute of Technology B.S. in Chemistry, June 2019

Pasadena, CA GPA: 4.0/4.0

## Experience

Graduate Student with Professor Mircea Dincă

2019 – present

MIT | Cambridge, MA

- Developed, synthesized, and characterized new sorbents for water capture at specific relative humidity
- Devised novel chemistry for post-synthetic modification of metal-organic frameworks
- Derived new chemical theory for structure-function relationships of capillary condensation
- Tackled issues of sustainability and cost by developing green synthetic methods
- Mentored two undergraduate students scientifically and professionally
- Managed international collaborative teams

# Research Assistant with Professor Harry Gray

2018 - 2019

Caltech | Pasadena, CA

· Utilized density functional theory and ab initio methods to resolve long-standing electronic structure problems

## Research Assistant with Professor William Goddard III

2016 - 2019

Caltech | Pasadena, CA

- Developed polarizable force fields for molecular simulations
- Utilized density functional theory methods to investigate reaction mechanisms including CO2 and CO upgrading

### Honors and Awards

Alan Davison Fellowship	2023
Department of Chemistry Award for Outstanding Teaching	2020 - 2021
ACS Undergraduate Award in Physical Chemistry	2019
Richard P. Schuster Memorial Prize	2019
George W. Housner Prize for Academic Excellence and Original Research	2019
George W. and Bernice E. Green Memorial Prize, Caltech	2018
Doris S. Perpall SURF Speaking Competition Semifinalist, Caltech	2017, 2018
Ernest H. Swift, Arthur A. Noyes, George R. Rossman SURF Fellow	2016, 2017, 2018

#### **Skills**

Driven by technical challenges • crystallography (powder and single crystal interpretation and refinement) • gas adsorption techniques • air-free chemical handling • spectroscopic characterizations and theory (infrared, UV-Vis, Raman, NMR, X-ray photoelectron) • computational methods (DFT, molecular dynamics) • magnetometry • instrument repair (high vacuum systems, high pressure systems, basic electronics) • Python • MS Excel and PowerPoint • Mathematica • Broadly interested in scientific communication, climbing, and 3D rendering

## Teaching

Physical Methods in Inorganic Chemistry (5.068, Grader)	2021, 2022, 2023
Inorganic Chemistry (5.04)	2020
General Chemistry (5.112)	2019

### Committee Service/Leadership

Environment, Health, and Safety Committee, MIT

2020 - present

Led level II laboratory inspections • recommended modifications to the Department of Chemistry Chemical Hygiene Plan and Safety Manual • well-versed in best practices for managing hazardous waste

MIT Chemistry Graduate Student Committee, Voting Member

2020 – present

#### **Talks**

Inorganic Chemistry Gordan Research Seminar

2022

Isolation of a Side-On V(III)- $(\eta^2-O_2)$  through the Intermediacy of a Low-V alent V(II) in a Metal-Organic Framework

## Coursework

Advanced Inorganic Chemistry (5.04, 5.05, 5.062, 5.068, Ch 102, 112, 153ab, 154, 213abc) • X-Ray Crystallography (5.067, 5.069) • Computational Chemistry (10.637) • Statistical Mechanics (127ab, 121abc) • Quantum Mechanics (Ph 125ab)

#### **Publications**

h-index: 13, i10-index: 16

\*first author (11 publications), ‡corresponding author

- 1. \*Tunable Low–Relative Humidity and High–Capacity Water Adsorption in a Bibenzotriazole Metal–Organic Framework. *Journal of the American Chemical Society*. (submitted).
- 2. A Solid Zn-Ion Conductor from an All-Zinc MOF Replete with Mobile Zn<sup>2+</sup> Cations. *Journal of the American Chemical Society.* (submitted).
- 3. A Layered Organic Cathode for High-Energy, Fast-Charging, and Long-Lasting Li-ion Batteries. ChemRxiv. 2023
- 4. Solid-State Investigation, Storage, and Separation of Pyrophoric PH<sub>3</sub> and P<sub>2</sub>H<sub>4</sub> with α-Mg Formate. *Angewandte Chemie*. **2023**. (3 citations)
- 5. Ultrafast Water H-Bond Rearrangement in a Metal-Organic Framework Probed by Femtosecond Time-Resolved Infrared Spectroscopy. *Journal of the American Chemical Society.* **2023**. (1 citation)
- 6. \*Conceptual and Practical Aspects of Metal-Organic Frameworks for Solid-Gas Reactions. *Chemical Reviews.* **2023**. (2 citations)
- 7. Reversible Topochemical Polymerization and Depolymerization of a Crystalline Three-Dimensional Porous Organic Polymer with C–C Bond Linkages. *Chem.* **2022**. (3 citations)
- 8. Pyrogallate-Based Metal-Organic Framework with a Two-Dimensional Secondary Building Unit, *Angewandte Chemie*. **2022**. (2 citations)
- 9. Room-Temperature Quantitative Quantum Sensing of Lithium Ions with a Radical-Embedded Metal-Organic Framework, *Journal of the American Chemical Society.* **2022**. (14 citations)
- 10. Thousand-fold increase in O2 electroreduction rates with conductive MOFs. ACS Central Science. 2022. (19 citations)
- 11. Dimensionality Modulates Electrical Conductivity in Compositionally Constance One-, Two-, and Three-Dimensional Frameworks. *Journal of the American Chemical Society.* **2022**. (14 citations)
- 12. Dipole-mediated exciton management strategy enabled by reticular chemistry. Chemical Science. 2022. (2 citations)
- 13. Strong magnetic exchange coupling in a radical-bridged trinuclear nickel complex. Dalton Transactions. 2022.
- \*Isolation of a Side-On V(III)-(η²-O₂) through the Intermediacy of a Low-Valent V(II) in a Metal–Organic Framework.
  *Inorganic Chemistry.* 2021. (2 citations)
- 15. \*Divergent Adsorption Behavior Controlled by Primary Coordination Sphere Anions in the Metal–Organic Framework Ni<sub>2</sub>X<sub>2</sub>BTDD. *Journal of the American Chemical Society.* **2021**. (13 citations)
- 16. Accelerated Synthesis of a Ni<sub>2</sub>Cl<sub>2</sub>(BTDD) Metal—Organic Framework in a Continuous Flow Reactor for Atmospheric Water Capture. ACS Sustainable Chemistry & Engineering. 2021. (24 citations)
- 17. \*Aperiodic Metal-Organic Frameworks. *Chemical Science.* **2020**. (**Most popular 2019-2020 inorganic, main group and crystal engineering chemistry articles**) (10 citations)
- 18. \*Catalytic Non-Redox Carbon Dioxide Fixation in Cyclic Carbonates. Chem. 2019. (71 citations)
- 19. \*‡Electronic Structure of Tetracyanonickelate (II). *Inorganic Chemistry*. **2019**. (**Most read Inorganic Chemistry article November 2019**) (9 citations)
- 20. Accurate Non-Bonded Potentials Based on Periodic Quantum Mechanics Calculations for Use in Molecular Simulations of Materials and Systems. *The Journal of Chemical Physics.* **2019**. (22 citations)
- 21. CO Coupling Chemistry of a Terminal Mo Carbide: Sequential Addition of Proton, Hydride, and CO Releases Ethenone. *Journal of the American Chemical Society.* **2019**. (30 citations)
- 22. Interface Structure in Li-Metal/[Pyr<sub>14</sub>][TFSI]-Ionic Liquid System from Ab Initio Molecular Dynamics Simulations. *The Journal of Physical Chemistry Letters.* **2019**. (28 citations)
- 23. \*Structures and Spectroscopic Properties of Metallocorrole Nanoparticles. *Inorganic Chemistry.* **2019**. (12 citations)
- 24. First-Principles—Based Reaction Kinetics from Reactive Molecular Dynamics Simulations: Application to Hydrogen Peroxide Decomposition. *PNAS*. **2018**. (35 citations)
- 25. \*Extension of the Polarizable Charge Equilibration Model to Higher Oxidation States with Applications to Ge, As, Se, Br, Sn, Sb, Te, I, Pb, Bi, Po, and At Elements. *The Journal of Physical Chemistry A.* **2018**. (17 citations)
- 26. \*Shock Synthesis of Five-Component Icosahedral Quasicrystals. Nature Scientific Reports. 2017. (21 citations)
- 27. \*Shock Synthesis of Decagonal Quasicrystals. Nature Scientific Reports. 2017. (25 citations)
- 28. Stem Cell Therapy and Curcumin Synergistically Enhance Recovery from Spinal Cord Injury. *PLOS ONE*. **2014**. (88 citations)

#### References

Prof. Mircea Dincă: mdinca@mit.edu (W. M. Keck Professor of Energy)

Dr. Peter Müller: pmueller@mit.edu (Principal Research Scientist)

Prof. Daniel Suess: suess@mit.edu (Class of '48 Career Development Assistant Professor of Chemistry)