Minsik Cho

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EDUCATION

Massachusetts Inst. of Technology / Doctoral Student in Chemistry

SEP 2022 – PRESENT CAMBRIDGE, MASSACHUSETTS

- Kwanjeong Fellow — SEP 2022 – MAY 2027
- Robert T. Haslam (1911) MIT Presidential Fellow — SEP 2022 – MAY 2023
- Head Graduate TA [5.601/5.602: Thermodynamics and Kinetics] — SEP 2022 – MAY 2023

Brown University / Sc. B. in Chemical Physics (w/ Honors; *magna cum laude*)

SEP 2016 – MAY 2022 PROVIDENCE, RHODE ISLAND

- Undergraduate Research, *Rubenstein Group* — DEC 2016 – MAY 2022
  - Studied strategies for expanding FT-AFQMC method into transition metals
  - Developed exact diagonalization code using `C++` & `lapack` to benchmark group's Finite-Temperature Auxiliary Field Quantum Monte Carlo method code *[1]
- Chemistry Teaching Assistant
  - CHEM330 [*Equilibrium, Rate, and Structure*] — SEP 2020 – DEC 2021
  - CHEM500 [*Inorganic Chemistry (Computational Lab)*] — JAN 2021 – APR 2021
- HPC Consultant at Center for Computation & Visualization — SEP 2019 – MAY 2022
- University Council of Students IT Advisory Board Member — JAN 2020 – DEC 2021
- Student Technician at Computing & Information Services — SEP 2016 – MAY 2017

RESEARCH / PROFESSIONAL EXPERIENCES

SURF-CTC Research Fellow / Gagliardi Group, University of Chicago

JUN 2021 – AUG 2021 CHICAGO, ILLINOIS

- Modeled CO-MgO(001) binding energy as one of the first applications of periodic density matrix embedding theory (pDMET) on realistic systems *[4]
- Studied ways to achieve parameter-less workflow for pDMET calculations

Google Summer of Code / OpenChemistry · `cclib`

JUN 2020 – SEP 2020 REMOTE

- Implemented four atomic partial charge methods (QTAIM, DDEC6, Hirshfeld, & Bickelhaupt) to expand `cclib`'s modern population analysis
- Wrote and updated bridges for interoperability with `horton` and `pyquante2`

Kupcinet-Getz Research Fellow / Martin Group, Weizmann Inst of Science

JUN 2019 – AUG 2019 REHOVOT, ISRAEL

- Assessed 24 atomic partial charge methods using principal component analysis on GMTKN55 set *[2] to provide a well-rounded guide method choice
- Parallelized group's serial script with `xargs` & `OpenMP` to improve efficiency *[3]

Unit Information Technology Specialist / Eighth United States Army

JUN 2017 – MAR 2019 TSAK, US ARMY GARRISON-HUMPHREYS, KOREA

- Provided IT support for Eighth Army simulators, training devices, & ranges
- Served as Platoon Senior KATUSA, counseling around 15 soldiers within the unit and assisting new enlisted soldiers through on-job trainings

PUBLICATIONS

*[1] Liu, Y.; **Cho, M.**; Rubenstein, B. Ab Initio Finite Temperature Auxiliary Field Monte Carlo. *Journal of Chemical Theory and Computation* **2018**, *14* (9), 4722-4732

*[2] **Cho, M.**; Sylvetsky, N.; Eshafi, S.; Santra, G.; Efremenko, I.; Martin, J. M. L. The Atomic Partial Charges Arboretum: Trying to See the Forest for the Trees. *ChemPhysChem* **2020**, *21* (8), 688-696

*[3] Santra, G.; **Cho, M.**; Martin, J. M. L. Exploring Avenues Beyond Revised DSD Functionals: I. Range Separation, with xDSD as a Special Case. *J. Phys. Chem A* **2021**, *125* (21), 4614-4627

*[4] Mitra, A.; Hermes, M.; **Cho, M.**; Agarawal, V.; Gagliardi, L. Periodic Density Matrix Embedding for CO Adsorption on the MgO(001) Surface. *J. Phys. Chem Lett.* **2022**, *13* (00), 7483-7489

HONORS

MIT Dept. of Chemistry Award for Outstanding Teaching
MIT Dept. of Chemistry

ACS Undergraduate Award in Physical Chemistry
ACS Division of Physical Chemistry

Paul Cross Prize in Chemistry
Brown University Dept. of Chemistry

Commendation of Excellence in Research
Brown University Dept. of Chemistry

Army Commendation Medal
DCG-S, Eighth U.S. Army

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EDUCATION

Massachusetts Institute of Technology / Doctoral Student in Chemistry — SEP 2022 – PRESENT

- Kwanjeong Fellow — SEP 2022 – MAY 2027
- Robert T. Haslam (1911) MIT Presidential Fellow — SEP 2022 – MAY 2023

CERTIFICATES

- MIT Research Mentoring Certificate — JAN 2024

Brown University / Bachelor of Science in Chemical Physics (with Honors, *magna cum laude*) — SEP 2016 – MAY 2022

- Advisors: Prof. Brenda Rubenstein (Research, Academic), Prof. Richard Stratt (Academic)
- University Council of Students IT Advisory Board Member — JAN 2020 – DEC 2021

ON CAMPUS (PART-TIME) JOBS

- HPC Consultant at Center for Computation & Visualization — SEP 2019 – MAY 2022
  - Maintained Brown's research cluster 'Oscar' as a member of HPC (High Performance Computing) Team. Written `bash` and `Python` scripts that monitor and store results in `MySQL` server for analysis of node performance. https://github.com/brown-ccv/osu-benchmarks
  - Led workshops introducing Brown's computing cluster to new researchers & benchmarked quantum chemistry packages on Oscar
- Student Technician at Computing & Information Services — SEP 2016 – MAY 2017

PUBLICATIONS

*1 Liu, Y.; **Cho, M.**; Rubenstein, B. Ab Initio Finite Temperature Auxiliary Field Monte Carlo. *Journal of Chemical Theory and Computation* **2018,** *14* (9), 4722-4732

*2 **Cho, M.**; Sylvetsky, N.; Eshafi, S.; Santra, G.; Efremenko, I.; Martin, J. M. L. The Atomic Partial Charges Arboretum: Trying to See the Forest for the Trees. *ChemPhysChem* **2020**, *21* (8), 688-696

*3 Santra, G.; **Cho, M.**; Martin, J. M. L. Exploring Avenues Beyond Revised DSD Functionals: I. Range Separation, with xDSD as a Special Case. *J. Phys. Chem A* **2021**, *125* (21), 4614-4627

*4 Mitra, A.; Hermes, M.; **Cho, M.**; Agarawal, V.; Gagliardi, L. Periodic Density Matrix Embedding for CO Adsorption on the MgO(001) Surface. *J. Phys. Chem Lett.* [Sub.] **2022**, *125* (21), 4614-4627

RESEARCH

SURF-CTC Research Fellow, Gagliardi Group (University of Chicago) — JUN 2021 – AUG 2021

- Modeling CO-MgO (001) Binding Energy using Periodic Density Matrix Embedding Theory (pDMET)
  - As one of the first few attempts in applying periodic density matrix embedding theory onto realistic systems, the binding energy of CO on MgO surface was modeled.
  - Working towards transforming periodic density matrix embedding theory into a blackbox-like workflow, I investigated simple yet parameter-less schemes for determining impurity orbitals from a set of localized orbitals.
  - Relevant Publication: *4

Undergraduate Researcher, Rubenstein Group (Brown University) — DEC 2016 – AUG 2021

- Field Sampling Techniques for Finite Temperature Auxiliary Field Monte Carlo (FT-AFQMC)
  - Studying how auxiliary field space can be efficiently sampled in the finite temperature realm to maintain desired accuracy while reducing computational costs. The motivation was to extend FT-AFQMC to complex systems i.e. transition metal complexes.
  - Karen T. Romer Undergraduate Teaching & Research Award — JUN 2020 – AUG 2020
- Exact Diagonalization Code
  - Written exact diagonalization code in C++, interfaced with Intel Math Kernel Library (MKL) lapack & BLAS routines, to provide benchmark values for the group's FT-AFQMC code during freshman year in college. For memory optimization, quantum states were expressed and propagated using bitwise operators.
  - Relevant Publication: *1

Google Summer of Code, with OpenChemistry & `cclib` JUN 2020 – AUG 2020

· Implementation of Modern Partial Charge Methods

- Implemented four new partial charge methods for Python-based quantum chemistry parser & analysis library. QTAIM, DDEC6, Hirshfeld, & Bickelhaupt methods were added to the existing code base. By contributing to a medium-sized opensource project, I learned to effectively understand existing code, write quality code that fits in the project, and utilize continuous integration (CI) tools for robust development. This work has also been a natural progression from the previous research at Weizmann. To efficiently evaluate charge densities and partition according to the gradients, `numpy` was extensively used for matrix operations.

· Addition & Updates for Bridges

- Added a new bridge from `pyquante2` and updated bridge to/from `horton` for interoperability with `cclib`.

Kupcinet-Getz Research Fellow, Martin Group (Weizmann Inst. of Science) JUN 2019 – AUG 2019

· Analysis of Partial Charge Methods

- Analyzed different partial charge methods by performing principal component analysis. Raw data set of partial charges obtained from DFT calculations was computed for a diverse chemical benchmark set, 'GMTKN55', for applicability to wider range of systems. Trends in the behavior of different methods with distinct underlying theories were identified, and suggestions on partial charge method choice was provided in published paper for chemists.
- Relevant Publication: *2

· Parallelization of Numerical Solver

- Parallelized group's numerical solver using OpenMP and `xargs`. Because the solver was mainly used to perform parameter sweep, parallelizable parts of the code were treated with simple OpenMP directives then a script with `xargs` calls were written for concurrent computation. This simple structure ensures maximal portability and minimal obscuring changes to the original code.
- Relevant Publication: *3

TEACHING

Teaching Assistant, *Thermodynamics and Kinetics* (5.601 & 5.602) SEP 2022 – MAY 2023

· Coordinated course logistics and managed distribution of workload among four course TAs as a Head TA (Fall 2022)

· Led two recitation sections weekly, written exams, and graded problem sets

Teaching Assistant, *Inorganic Chemistry Lab* (CHEM500L) JAN 2021 – APR 2021

· Tutored computational chemistry lab section that utilized `orca` to perform DFT calculations (geometry optimization and properties evaluation) on transition metal complexes bound with SNO ligands. The lab was a HHMI-funded CURE (Course-based Undergraduate Research Experience) component.

· Maintained Slack chat rooms to provide a robust support network for students during remote instruction of labs

Teaching Assistant, *Equilibrium, Rate, and Structure* (CHEM330) SEP 2020 – DEC 2021

· Taught about 15 students in weekly group problem sessions. The sessions reviewed the concepts introduced in the introductory chemistry course lecture and reinforced understanding by solving problems in a group setting.

HONORS, FELLOWSHIPS, & FUNDING

· **MIT Department of Chemistry Award for Outstanding Teaching** AUG 2023

· **MIT Presidential Fellowship** Robert T. Haslam (1911) Presidential Fellowship SEP 2022

· **Kwanjeong Fellowship** JUL 2022

· **ACS PHYS Undergraduate Award in Physical Chemistry** MAY 2022

· **Paul Cross Prize in Chemistry** MAY 2022

· **Commendation of Excellence in Research** MAY 2022

· **SURF-CTC Summer Research Fellowship** JUN 2021

· **Karen T. Romer Undergraduate Teaching and Research Award** JUN 2020

· **Kupcinet-Getz Summer Research Fellowship** JUN 2019

· **Brown University Financial Aid**

- JY Kwak '16 Scholarship Fund & Shoman Scholarship Fund 2021-2022
- JY Kwak '16 Scholarship Fund 2020-2021
- Brown University Scholarship 2019-2020, 2016-2017

- **Army Commendation Medal (ARCOM),** Deputy Commanding General-Sustainment, Eighth United States Army MAR 2019

SERVICE

- **MIT ACCESS Student Panel** (Diversity Event at MIT Chemistry) OCT 2023
- **Chemistry Application Mentor Program Mentor** (Assistance for applicants from underrepresented backgrounds) OCT 2023
- **Teaching Training Facilitator,** MIT Chemistry Graduate Student Orientation AUG 2023
- **Peer Mentor,** MIT Chemistry Peer Mentorship Program 2023-2024
- **Panelist,** International Student Internships in Focus: STEM Panel, Brown University MAR 2022
- **Science Fair Judge,** Times Squared Academy, Providence RI FEB 2020