

Education

2022 – Current **Ph.D.**, Chemistry, Massachusetts Institute of Technology
2016 – 2022 **Sc.B.**, Chemical Physics (with Honors, *magna cum laude*), Brown University

Research Experience

2022 – Current Graduate Research Assistant, MIT, (Advisor: [Troy Van Voorhis](#))
2016 – 2022 Undergraduate Researcher, Brown University (Advisor: [Brenda Rubenstein](#))
2021 SURF-CTC Summer Research Fellow, University of Chicago (Advisor: [Laura Gagliardi](#))
2019 Kupcinet-Getz Summer Research Fellow, Weizmann Institute of Science
 (Advisor: [Gershon Martin](#))

Awards & Honors

Aug 2023 MIT Department of Chemistry Award for Outstanding Teaching
Sep 2022 MIT Presidential Fellowship [Robert T. Haslam (1911) Fellow]
Jul 2022 Kwanjeong Fellowship
May 2022 ACS PHYS Undergraduate Award in Physical Chemistry
May 2022 Paul Cross Prize in Chemistry
May 2022 Commendation of Excellence in Research
Jun 2020 Karen T. Romer Undergraduate Teaching & Research Award
Mar 2019 Army Commendation Medal (ARCOM)

Publications

 [Google Scholar](#)

† Equal contribution

Journal Articles

- J1. Berquist, E., Dumi, A., Upadhyay, S., Abarbanel, O. D., **Cho, Minsik**, Guar, S., Gil, V. H. C., Hutchison, G. R., Lee, O. S., Rosen, A. S., Schamnad, S., Schneider, F. S. S., Steinmann, C., Stolyarchuk, M., Vandezande, J. E., Zak, W. & Langner, K. M. cclib 2.0: An Updated Architecture for Interoperable Computational Chemistry. *The Journal of Chemical Physics* **161**, 042501 (2024).
- J2. Erakovic, M., Witteveen, F., Harley, D., Günther, J., Bensberg, M., Meitei, O. R., **Cho, Minsik**, Van Voorhis, T., Reiher, M. & Christandl, M. High ground state overlap via quantum embedding methods. *PRX Life* (2024). arxiv:2408.01940.
- J3. Tran, H. K., Weisburn, L. P., **Cho, Minsik**, Weatherly, S., Ye, H.-Z. & Van Voorhis, T. Bootstrap Embedding for Molecules in Extended Basis Sets. *Journal of Chemical Theory and Computation* (2024).

- J4. Mitra, A., Hermes, M. R., **Cho, Minsik**, Agarwal, V. & Gagliardi, L. Periodic Density Matrix Embedding for CO Adsorption on the MgO(001) Surface. *The Journal of Physical Chemistry Letters* **13**, 7483–7489 (2022).
- J5. Santra, G., **Cho, Minsik** & Martin, J. M. L. Exploring Avenues beyond Revised DSD Functionals: I. Range Separation, with xDSD as a Special Case. *The Journal of Physical Chemistry A* **125**, 4614–4627 (2021).
- J6. **Cho, Minsik**, 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* **21**, 688–696 (2020).
- J7. Liu, Y., **Cho, Minsik** & Rubenstein, B. Ab Initio Finite Temperature Auxiliary Field Quantum Monte Carlo. *Journal of Chemical Theory and Computation* **14**, 4722–4732 (2018).

Working Papers

- W1. Weisburn, Leah P.[†], **Cho, Minsik**[†], Bensberg, M., Meitei, O. R., Reiher, M. & Van Voorhis, T. *Multiscale Embedding for Quantum Computing* 2024. arxiv:2409.06813.

Presentations

Talks

- T1. **Cho, Minsik** & Van Voorhis, T. *Partially Updated Bootstrap Embedding*. American Chemistry Society (ACS) Fall 2024 (Contributed; Denver, CO). Aug. 2024.
- T2. **Cho, Minsik**[†], Weisburn, Leah P.[†] & Van Voorhis, T. *Quantum Chemistry with Limited Quantum Resources Using Bootstrap Embedding* (제한된 양자 컴퓨터 자원을 이용한 양자 화학 계산: Bootstrap Embedding 기반 전략). Samsung Advanced Institute of Technology (SAIT) Simulation Society (Invited; Suwon, Korea). July 2024.

Teaching

Massachusetts Institute of Technology

- Jan 2024 MIT Professional Development Certificate in Research Mentoring
- Spring 2023 Teaching Assistant, Thermodynamics and Kinetics (5.601 & 5.602)
- Fall 2022 Head Teaching Assistant, Thermodynamics and Kinetics (5.601 & 5.602)

Brown University

- Spring 2021 Teaching Assistant, Inorganic Chemistry (CHEM500) Computational Lab
- Fall 2020, Spring 2020, and Fall 2021 Teaching Assistant, Equilibrium, Rate, and Structure (CHEM330)

Software

QuEmb

One of the main developers for [QuEmb](#), a Python package developed in the Van Voorhis Group for Bootstrap Embedding calculations.

cclib

Contributed to the development of [cclib](#), a Python-based parsing and postprocessing library for computational chemistry workflows. Participated in the Google Summer of Code 2020.

Service

2024 – Current	Organizer, Greater Boston Area Theoretical Chemistry (Theochem) Seminar Series
2023 – 2024	Teaching Assistants Training (Graduate Student Orientation) Facilitator
2023 – 2024	MIT Chemistry Peer Mentorship Program Mentor
2023	MIT ACCESS Student Panel
2023	MIT Chemistry Application Mentor Program (CAMP) Mentor
2022	Panelist, Brown University International Student Internships in Focus: STEM
2020 – 2021	University Council of Students (UCS) IT Advisory Board Member
2020	Science Fair Judge, Times Squared Academy (Providence, RI)

Other Experience

2019 – 2022	High Performance Computing Consultant, Center for Computation and Visualization
2017 – 2019	Unit Information Technology Specialist & Platoon Senior KATUSA, Eighth US Army
2016 – 2017	Student Technician, Computing and Information Services

Last updated: December 18, 2024