Henry K. Tran

3000 Broadway, 138 Havemeyer Hall, New York, NY 10027

☎ (212) 854-2202 ◇ ✉ hkt2112@columbia.edu

Professional Experience

Postdoctoral Scientist, Columbia University, New York, NY, USA — *Sep 2022–Present*
Advisor: Timothy C. Berkelbach (✉ t.berkelbach@columbia.edu)

Education

PhD Chemistry, Massachusetts Institute of Technology, Cambridge, MA, USA — *Aug 2017–Sep 2022*
Advisor: Troy A. Van Voorhis (✉ tvan@mit.edu)

MPhil Scientific Computing, University of Cambridge, Cambridge, UK — *Sep 2016–Sep 2017*
Advisor: Alexander J. W. Thom (✉ ajwt3@cam.ac.uk)

BS Mathematics and Chemistry, The Ohio State University, Columbus, OH, USA — *Aug 2012–May 2016*
Advisor: Terry A. Miller (✉ tamiller@chemistry.ohio-state.edu)

Publications (Google Scholar)

6. H.-Z. Ye, **H. K. Tran**, T. Van Voorhis. "Accurate Electronic Excitation Energies in Full-Valence Active Space via Bootstrap Embedding," *J. Chem. Theory Comput.* 2021, 17, 3335–3347.
5. **H. K. Tran**, H.-Z. Ye, T. Van Voorhis. "Bootstrap Embedding with an Unrestricted Mean-Field Bath," *J. Chem. Phys.* 2020, 153, 214101.
4. H.-Z. Ye, **H. K. Tran**, T. Van Voorhis. "Bootstrap Embedding for Large Molecular Systems," *J. Chem. Theory Comput.* 2020, 16, 5035–5046.
3. H.-Z. Ye, N. D. Ricke, **H. K. Tran**, T. Van Voorhis. "Bootstrap Embedding for Molecules," *J. Chem. Theory Comput.* 2019, 15, 4497–4506.
2. **H. K. Tran**, T. Van Voorhis, A. J. W. Thom. "Using SCF Metadynamics to Extend Density Matrix Embedding Theory to Excited States," *J. Chem. Phys.* 2019, 151, 034112.
1. **H. K. Tran**, J. F. Stanton, T. A. Miller. "Quantifying the effects of higher order coupling terms on fits using a second order Jahn-Teller Hamiltonian," *J. Mol. Spec.* 2018, 343, 102–115.

Submitted and In Preparation

4. **H. K. Tran**, T. C. Berkelbach. "Semistochastic vibrational heat-bath configuration interaction with a VSCF reference," *in preparation*
3. **H. K. Tran**, T. Van Voorhis. "Fundamental Band Gaps of Graphene Quantum Dots and Organic Polymers using Bootstrap Embedding," *in preparation*
2. **H. K. Tran**, T. Van Voorhis. "Bootstrap Embedding augmented with Pair Natural Orbitals," *in preparation*
1. **H. K. Tran**, H.-Z. Ye, T. Van Voorhis. "Bootstrap Embedding for Molecules in Extended Basis Sets," *in preparation*

Research Projects

Columbia University | Advisor: Timothy C. Berkelbach

◇ **Anharmonic Vibrational Structure Theory** — *2022 – Present*

- Derived and implemented heat-bath CI criterion for vibrational Hamiltonians based on harmonic oscillator product states and VSCF modal product states. Applied Einstein-Nesbet perturbation corrections for vibrational systems.

Massachusetts Institute of Technology | Advisor: Troy A. Van Voorhis

◇ **Electron Correlation with Quantum Embedding** *2017 – 2022*

- Developed and implemented fragment based pair natural orbital (PNO) theory for Bootstrap Embedding (BE) to capture dynamic correlation in fragment embedding. Demonstrated the ability of fragment based PNOs to systematically improve embedding without increasing fragment size.
- Developed and implemented various orbital localization schemes for use in BE. Improved convergence and accuracy of BE calculations for molecular systems in large basis sets (6-311G and cc-pVDZ) to less than 1% error.
- Generalized and implemented Density Matrix Embedding Theory (DMET) and BE to spin unrestricted systems. Applied these methods to model excited states, singlet-triplet gaps, ionization potentials, electron affinities, and band gaps to less than 1% error.
- Worked with three graduate students and one postdoctoral researcher. Mentored one graduate student.

◇ **Calculations of Core Electron Binding Energies using MPn** *2021 – 2022*

- Implemented unrestricted and restricted open-shell MP2 and MP3 for calculation of doublet states.
- Benchmarked ΔMP2 and ΔMP3 against ΔCCSD for the prediction of core electron binding energies. Correlation versus ΔCCSD was considered and an R value of up to 0.99943 was found for small molecules.
- Implemented and tested local fragment embedding methods for prediction of core electron binding energies.
- Worked with and mentored one undergraduate student and one graduate student.

University of Cambridge | Advisor: Alexander J. W. Thom

◇ **Quantum Embedding from Higher-Lying Mean-Field Baths** *2016 – 2017*

- Generalized and implemented DMET starting from bath states obtained from higher lying SCF metadynamics solutions to predict excited state energies via quantum embedding.

The Ohio State University | Advisor: Terry A. Miller

◇ **Rovibronic Analysis of the $\widetilde{A}^2E'' \leftarrow \widetilde{X}^2A_2'$ Transition of NO_3** *2013 – 2016*

- Derived and implemented a rovibronic Hamiltonian model for the rovibronic transitions of NO_3, including coriolis coupling, spin-orbit coupling, spin-rotation coupling, and Jahn-Teller coupling.
- Modeled the rotational structure of the vibronic bands in the $\widetilde{A}^2E'' \leftarrow \widetilde{X}^2A_2'$ transition to within experimental error. Determined rovibronic Hamiltonian parameters through empirical fits, and identified negligible Jahn-Teller coupling.

◇ **Jahn-Teller Coupling in the $\tilde{X}^2E'$ Electronic State of Li_3** *2015 – 2016*

- Derived and implemented a parametrized vibronic Hamiltonian model. Determined the magnitude of Jahn-Teller coupling in the vibrational spectrum of Li_3.
- Proposed and conducted an analysis to determine the limitations of fitting second order Jahn-Teller Hamiltonians to systems with significant fourth order Jahn-Teller coupling.

Honors and Awards

◇ **NSF Graduate Research Fellow** (1 of 2048 | Natl.) *2017 – 2021*
National Science Foundation

◇ **MIT Chemistry Outstanding Teaching Award** (1 of 17 | Dept.) *2017 – 2018*
Dept. of Chemistry, MIT — For dedication to teaching duties in 5.61 and 5.111.

- ◇ **Churchill Scholar** (1 of 15 | Natl.) *2016 – 2017*
  Winston Churchill Foundation of the United States
- ◇ **Barry M. Goldwater Scholar** (1 of 260 | Natl.) *2015 – 2016*
  Excellence in Education Foundation
- ◇ **Top Sophomore, Junior, Senior in Chemistry** (1 of 1 | Dept.) *2014 – 2016*
  Dept. of Chemistry and Biochemistry, OSU
- ◇ **Undergraduate Research Scholarship** (1 of 60 | Coll.) *2014 – 2016*
  College of Arts and Sciences, OSU — Research grant. Top award. Awarded twice.
- ◇ **Gary Booth Scholarship** (1 of 10 | Dept.) *2014 – 2016*
  Dept. of Chemistry and Biochemistry, OSU — For academic merit in chemistry.
- ◇ **Morrill Excellence Scholar** (1 of 300 | Natl.) *2012 – 2016*
  Office of Diversity and Inclusion, OSU — For diversity based leadership.
- ◇ **Undergraduate Mathematics Scholarship** (Dept.) *2013 – 2015*
  Dept. of Mathematics, OSU — For academic merit in mathematics.

Selected Presentations

Oral Presentations

5. **H. K. Tran**, T. Van Voorhis, A. J. W. Thom. "Direct Embedding of Excited States using Density Matrix Embedding Theory," In: 257$^{\text{th}}$ American Chemical Society National Meeting, Orlando, FL, USA, March 31–April 4, 2019.
4. **H. Tran**, T. A. Miller. "Analysis of the Rotationally Resolved Non-Degenerate (a_1'') and Degenerate (e') Vibronic Bands in the $\widetilde{A}^2E'' \leftarrow \widetilde{X}^2A_2'$ Transition of NO_3," In: *71th International Symposium on Molecular Spectroscopy*, Champaign-Urbana, IL, USA, June 20–24, 2016.
3. **H. Tran**, J. F. Stanton, T. A. Miller. "Quantifying the Effects of Higher Order Jahn-Teller Coupling Terms on a Quadratic Jahn-Teller Hamiltonian in the Case of NO_3 and Li_3," In: *71th International Symposium on Molecular Spectroscopy*, Champaign-Urbana, IL, USA, June 20–24, 2016.
2. **H. Tran**, T. A. Miller. "Analysis of the Rotationally Resolved Spectra to the Degenerate (e') Upper-State Vibronic Levels in the $\widetilde{A}^2E'' \leftarrow \widetilde{X}^2A_2'$ Electronic Transition of NO_3," In: *70th International Symposium on Molecular Spectroscopy*, Champaign-Urbana, IL, USA, June 22–26, 2015.
1. **H. Tran**, T. Codd, D. Melnik, M. Roudjane, T. A. Miller. "Rovibronic Analysis of the e' Bands in the $\widetilde{A}^2E''$ State of NO_3 Radical," In: *69th International Symposium on Molecular Spectroscopy*, Champaign-Urbana, IL, USA, June 16–20, 2014.

Poster Presentations

3. **H. K. Tran**, H.-Z. Ye, T. Van Voorhis. "Dynamic Correlation with Quantum Embedding," In: *American Conference on Theoretical Chemistry*, Olympic Valley, CA, USA, July 25–28, 2022.
2. **H. K. Tran**, H.-Z. Ye, T. Van Voorhis. "Bootstrap Embedding for Large Basis Sets," In: *12th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2020)*, Vancouver, BC, Canada, July 3–8, 2022.
1. **H. Tran**, M. Roudjane, T. J. Codd, M-W. Chen, D. G. Melnik, T. A. Miller, J. F. Stanton. "Analysis of the Rotationally Resolved Spectra in the $\widetilde{A}^2E'' \leftarrow \widetilde{X}^2A_2'$ Electronic Transition in the NO_3 Radical," In: *33rd International Symposium on Free Radicals*, Olympic Valley, CA, USA, August 2–7, 2015.

Teaching

- [**MIT**] **5.73** - Quantum Mechanics I (Graduate Level) — Grader *Autumn 2018*
  - Graded homework and exams. Wrote answer keys. Held weekly office hours. Wrote complementary Python scripts to visualize course material.
- [**MIT**] **5.111** - Principles of Chemical Science — Lab Demo TA (*won teaching award*) *Spring 2018*
  - Prepared lecture material and handouts for recitations held twice per week. Held office hours twice per week. Proctored exams. Graded homework and exams. Attended weekly TA meetings.
  - Further responsibilities as Lab Demo TA included preparing samples for demos used in lecture and cleaning up after demos.
- [**MIT**] **5.61** - Physical Chemistry — Head TA (*won teaching award*) *Autumn 2017*
  - Prepared lectures and handouts for recitations held twice per week. Held office hours twice per week. Wrote exam questions and proctored exams. Wrote homework and exam answer keys. Graded homework and exams. Attended weekly TA meetings. Typeset answer keys for OCW.
  - Further responsibilities as Head TA included distributing workload, reserving rooms for special lectures, running extra review sessions, filing paperwork for TA expenses.
- [**OSU**] **Chemistry 1210** - General Chemistry I — Lab TA *Autumn 2014*
  - Prepared necessary samples and equipment for lab sessions. Attended to students during lab sessions to maintain safety and cleanliness standards. Graded lab reports and assignments.

Students Supervised

- Ezra Alexander (MIT Graduate Student) *2022 – 2022*
- Anton Morgunov (MIT Undergraduate Student) *2022 – 2022*
- Leah Weisburn (MIT Graduate Student) *2021 – 2022*
- Yu-Che Chien (MIT Undergraduate Student) *2021*

Mentorship

- **STIMULUS Volunteer** (at The Grove Primary School) *2016 – 2017*
  - Served as assistant to classroom teacher.
  - Designed experimental programming curriculum for Year 5 students. Taught programming using `scratch` in a small group setting.
- **OSU Undergraduate Research Office Peer Research Contact** *2015 – 2016*
  - Provided one-on-one advising to undergraduates interested in chemistry and mathematics research.
  - Served on panels promoting undergraduate research.
- **OSU Arts and Science Honors Peer Mentor** *2013 – 2016*
  - Prepared lectures for undergraduate survey course. Supervised all lectures. Held biweekly office hours. Attended weekly mentor training.
  - Provided general academic advising to incoming freshmen. Organized social events.
- **OSU Office of Diversity and Inclusion Peer Mentor** *2014 – 2015*
  - One-on-one mentoring with freshmen belonging to underrepresented minority groups. Maintained regular monthly meetings and constant electronic communication.

Service

- **MIT Graduate Student Council (GSC)** — Activities Chair *and more* *2018 – 2022*
  - As Activities Committee Chair (2019 – 2021): Organized and supervised large scale events for graduate students to promote work-life balance and mental health well-being. Managed finances. Distributed tasks among committee members. Collaborated with Harvard Graduate Council.

- As Funding Board Rep. (2019 – 2021): Reviewed funding requests from all student groups.
- As Executive Committee (2019 – 2021): Scheduled meetings with GSC and MIT administration to discuss issues concerning graduate students, e. g., Epstein letters and COVID policies.

◇ **MIT Ashdown House Officer** — Brunch and Communities Chair *2018 – 2022*

- As Brunch Chair (2018 – 2020): Budgeted, organized, and supervised monthly dorm brunch social serving over 300 students. Applied for funding. Managed committee of 15 members.
- As Communities Chair (2020 – 2022): Budgeted, organized, and supervised various small group events within the dorm. Managed committee of 10 members.

◇ **GBA Theoretical Chemistry Seminar** — Organizer *2017 – 2022*

- Hosted one or two speakers each year. Sent invitations to potential speakers, served as first point of contact, booked flights and hotels for speaker, scheduled meetings between speaker and interested faculty/students, hosted seminar at MIT, organized thank you dinners.

◇ **Assistant Session Chair**, 71st Int. Symposium on Molecular Spectroscopy *2016*

- Provided technical support. Helped introduce speakers and enforced time limits on presentations.