Henry K. Tran

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Research Interests

Developing and applying a unified predictive framework for electron-phonon dynamics, leveraging quantum embedding, machine learning, and tensor networks to design next-generation materials for quantum information and clean energy.

Professional Appointments

Assistant Professor, Department of Chemistry, Mississippi State University — *Jul 2026–Present*

Postdoctoral Scientist, Columbia University, New York, NY, USA — *Sep 2022–Jul 2026*
Advisor: Timothy C. Berkelbach (✉ tcb2112@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)

Honors and Awards

- **NSF Graduate Research Fellow** (1 of 2048 | Natl.) — *2017 – 2021*
- **Churchill Scholar** (1 of 15 | Natl.) — *2016 – 2017*
- **Barry M. Goldwater Scholar** (1 of 260 | Natl.) — *2015 – 2016*

Publications (Google Scholar)

11. **H. K. Tran**, T. C. Berkelbach. "Exact mid-IR quantum vibrational spectra of neutral water clusters," *arXiv:2509.13517. submitted: J. Phys. Chem. Lett.* (2025)

10. M. Cho, O. R. Meitei, L. P. Weisburn, O. Weser, S. Weatherly, A. Alexiu, B. Hanscam, **H. K. Tran**, H.-Z. Ye, M. Welborn, N. Ricke, T. Tsuchimochi, A. Trofimov, T. Orkhon, N. Whelpley, C. Luo, T. Van Voorhis. "QuEmb: A Toolbox for Bootstrap Embedding Calculations of Molecular and Periodic Systems," *J. Phys. Chem. A.* 28, 6538–6551 (2025)

9. **H. K. Tran**, L. P. Weisburn, M. Cho, S. Weatherly, H.-Z. Ye, T. Van Voorhis. "Bootstrap Embedding for Molecules in Extended Basis Sets," *J. Chem. Theory Comput.* 20, 10912–10921 (2024)

8. A. Morgunov, **H. K. Tran**, O. R. Meitei, Y.-C. Chien, T. Van Voorhis. "MP2-based composite extrapolation schemes can predict core-ionization energies for first-row elements with coupled-cluster level accuracy," *J. Phys. Chem. A.* 128, 1089–5639 (2024)

7. **H. K. Tran**, T. C. Berkelbach. "Vibrational heat-bath configuration interaction with semistochastic perturbation theory using harmonic oscillator or VSCF modals," *J. Chem. Phys.* 159, 194101 (2023)

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.* 17, 3335–3347 (2021)

5. **H. K. Tran**, H.-Z. Ye, T. Van Voorhis. "Bootstrap Embedding with an Unrestricted Mean-Field Bath," *J. Chem. Phys.* 153, 214101 (2020)

4. H.-Z. Ye, **H. K. Tran**, T. Van Voorhis. "Bootstrap Embedding for Large Molecular Systems," *J. Chem. Theory Comput.* 16, 5035–5046 (2020)

3. H.-Z. Ye, N. D. Ricke, **H. K. Tran**, T. Van Voorhis. "Bootstrap Embedding for Molecules," *J. Chem. Theory Comput.* 15, 4497–4506 (2019)

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.* 151, 034112 (2019)

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.* 343, 102–115 (2018)

In Preparation

2. **H. K. Tran**, L. P. Weisburn, T. Van Voorhis. "Fundamental Band Gaps of Graphene Quantum Dots and Organic Polymers using Bootstrap Embedding," *in preparation*

1. **H. K. Tran**, L. P. Weisburn, T. Van Voorhis. "Bootstrap Embedding augmented with Pair Natural Orbitals," *in preparation*

Selected Presentations

Oral Presentations

6. **H. K. Tran**, T. C. Berkelbach. "Anharmonic Vibrational Structure and Spectra using Vibrational Heat-Bath Configuration Interaction," In: *5^{th} Theory and Applications of Computational Chemistry*, Hokkaido University, Sapporo, Japan, September 4–9, 2023.

5. **H. K. Tran**, T. Van Voorhis, A. J. W. Thom. "Direct Embedding of Excited States using Density Matrix Embedding Theory," In: *257^{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: *71^{th} 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: *71^{th} 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: *70^{th} 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: *69^{th} International Symposium on Molecular Spectroscopy*, Champaign-Urbana, IL, USA, June 16–20, 2014.

Poster Presentations

4. **H. K. Tran**, T. C. Berkelbach. "Exact Theoretical Vibrational Spectra using Tensor Decompositions and Selected CI," In: *American Conference on Theoretical Chemistry*, Chapel Hill, NC, USA, June 17–20, 2024.

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: *12^{th} 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: *33^{rd} International Symposium on Free Radicals*, Olympic Valley, CA, USA, August 2–7, 2015.

Research Experience and Key Accomplishments

Columbia University | Advisor: Timothy C. Berkelbach

- Architected and implemented a new paradigm for anharmonic vibrational spectroscopy by adapting selected configuration interaction (SCI) methods to the vibrational problem utilizing dimensionality reduction and stochastic sampling algorithms, enabling benchmark calculations with near-spectroscopic accuracy.
- Invented a novel, exact representation of the potential energy surface (PES) using Tensor Cross Interpolation (TCI) reducing memory complexity from exponential to linear, creating the core technology for Thrust 3 of my independent research program.
- Developed a direct spectral simulation technique that achieved a 100-fold speedup over diagonalization-based methods, leading to the most accurate theoretical vibrational spectra of water clusters to date.
- Engineered high-efficiency workflows integrating and training machine learning potentials (based on UMA, MACE) to achieve ab initio accuracy at a fraction of the computational cost, extending accessible dynamical simulation timescales by orders of magnitude.

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

- Conceived and led the development of a scalable quantum embedding framework that extended high-level accuracy to systems of hundreds of atoms, providing the foundational methodology for Thrust 1 and Thrust 2 of my independent research program.
- Directed the first extension of Bootstrap Embedding (BE) to excited states, enabling calculations of band gaps in large systems like graphene quantum dots.
- Initiated and led the development of the open-source QuEmb codebase, a robust scientific tool now used by multiple research groups.

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

- Conceived and implemented the first-ever extension of Density Matrix Embedding Theory (DMET) to excited states. This work uniquely utilized mean-field excited states as an effective bath, enabling the calculation of accurate potential energy surfaces with the efficiency of a quantum embedding approach.

The Ohio State University | Advisor: Terry A. Miller

- Resolved a decades-long controversy in atmospheric chemistry regarding the Jahn-Teller (JT) coupling in the NO_3 radical. Developed a novel model JT Hamiltonian that enabled the first-ever rotational analysis, definitively showing negligible JT coupling.

Teaching

- **OCW Course Developer** — 5.61 Physical Chemistry, MIT *Autumn 2017*
  Devised a syllabus suitable for the general public and developed notes and assignments for the MIT OCW 5.61 course. Published material and lecture videos to increase access to chemistry regardless of social or economic barriers.
- **Heading Teaching Assistant** — 5.61 Physical Chemistry, MIT *Autumn 2017*
  Led a team of TAs for a core undergraduate physical chemistry course. Developed and delivered weekly recitations, wrote exam questions and answer keys, and coordinated all TA duties. Received MIT Chemistry Outstanding Teaching Award for this role.
- **Teaching Assistant** — 5.111 Principles of Chemical Science, MIT *Spring 2018*
  Taught weekly recitation sections for a large introductory chemistry course. Prepared lecture materials and handouts, held office hours, and graded assignments. Received MIT Chemistry Outstanding Teaching Award for this role.

- **Grader** — 5.73 Quantum Mechanics I, MIT *Autumn 2018*
  Graded homework and exams for a graduate-level quantum mechanics course. Developed complementary Python scripts to help students visualize abstract concepts.
- **Lab Teaching Assistant** — Chemistry 1210 General Chemistry I, OSU *Autumn 2014*

Mentoring and Supervision

Research Mentorship

- **Anton Morgunov** (MIT Undergraduate Student, now PhD Student at Yale) *2022 – 2022*
  Supervised research on core-level spectroscopy methods, leading to a co-authored publication.
- **Leah Weisburn** (MIT Graduate Student) *2021 – 2022*
  Mentored on projects developing quantum embedding.
- **Yu-Che Chien** (MIT Undergraduate Student, now PhD Student at Stanford) *2021*
  Supervised research on core-level spectroscopy methods, leading to a co-authored publication.
- **OSU Undergraduate Research Office** — Peer Research Contact *2015 – 2016*
  Provided one-on-one advising to undergraduates seeking research opportunities in STEM fields.

Outreach and Community Engagement

- **MIT Chemistry Outreach Program** — Volunteer *2017 – 2018*
  Developed and presented engaging science demonstrations for students in under-served New England primary schools.
- **OSU Office of Diversity and Inclusion** — Peer Mentor *2014 – 2015*
  Provided one-on-one mentoring to first-year undergraduates from underrepresented minority groups, offering guidance on the academic and social transition to university life.

Professional Service and Leadership

- **GBA Theoretical Chemistry Seminar** — Organizer *2017 – 2022*
  Recruited and hosted internationally renowned speakers to foster a vibrant intellectual community among theoretical chemistry students and faculty at MIT, Harvard, and surrounding universities.
- **MIT Graduate Student Council (GSC)** — Chair *and more* *2018 – 2022*
  Led a committee to organize large-scale social and academic events for the 7,000+ graduate student community to foster interdepartmental collaboration and support student well-being. Managed a significant annual budget and collaborated with university administration.

References

- **Prof. Timothy C. Berkelbach**, *Associate Professor of Chemistry*
  Department of Chemistry, Columbia University
  Postdoctoral Advisor ◇ ☎ 212-854-2202 ◇ ✉ tcb2112@columbia.edu
- **Prof. Troy A. Van Voorhis**, *Department Head and Haslam and Dewey Professor of Chemistry*
  Department of Chemistry, Massachusetts Institute of Technology
  PhD Advisor ◇ ☎ 617-253-1488 ◇ ✉ tvan@mit.edu (Direct requests to: miaoli@mit.edu)
- **Prof. Alexander J. W. Thom**, *University Professor of Theoretical Chemistry*
  Department of Chemistry, University of Cambridge
  MPhil Advisor ◇ ☎ 01223 336470 ◇ ✉ ajwt3@cam.ac.uk