

HSIN-YU KO, PH.D.

Department of Chemistry, University of North Texas, Denton, Texas 76201 USA

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EDUCATION

Ph.D. in Theoretical Chemistry, Princeton University 2019

Thesis: *First-Principles Study on the Structural and Thermal Properties of Molecular Crystals and Liquids*

Advisor: Roberto Car

B.S. in Chemistry (*summa cum laude*), National Taiwan University 2010

Advisor: Bih-Yaw Jin

ACADEMIC EXPERIENCE

Assistant Professor, University of North Texas 09/2024 – present

Research: The Ko group studies atomistic structures and reactive processes of condensed-phase systems relevant to energy, materials, and environmental sciences. Based on quantum and statistical mechanics, we develop computational algorithms and software using high-performance computing and machine-learning techniques. Our applications cover many scopes of chemistry, e.g.: (1) designing next-generation fuel cells; (2) developing protocols to treat aqueous forever chemicals; (3) understanding structures and reactive processes of polymers.

Postdoctoral Research Associate, Cornell University 07/2019 – 08/2024

Advisor: Robert A. DiStasio Jr.

Postdoctoral Research Associate, Princeton University 02/2019 – 06/2019

Advisor: Roberto Car

Research Assistant, National Taiwan University 08/2011 – 07/2012

Advisor: Bih-Yaw Jin

HONORS & AWARDS

Membership (by nomination), Sigma Xi, The Scientific Research Honor Society 2025

Junior Faculty Summer Research Support Award, University of North Texas 2025

DCOMP Travel Award, APS March Meeting 2024

NERSC Early Career Award for High Impact Scientific Achievement, DOE/NERSC 2020

Pickering Teaching Award, Princeton University 2016

Chemistry Graduate Student Travel Grant, Princeton University 2015

Natural Sciences and Engineering Fellowship, Princeton University 2013

Studying Abroad Scholarship, Ministry of Education of Taiwan 2012

Research Poster Award, Chinese Chemical Society 2011

Phi Tau Phi Scholastic Honor Society, Taiwan 2010

Dean's Award, National Taiwan University 2010

Research Poster Award, National Taiwan University 2010

COMPUTER RESOURCE ALLOCATIONS/AWARDS

UNT Research Project (18,000 Lonestar6-SU and 1,00 Vista-SU, PI), TACC 2026

UNT Research Project (12,300 Lonestar6-SU and 1,000 Vista-SU, PI), TACC 2025

Energy Research Computing Allocations ($\approx$ 4M CPU Hours/year, PI), DOE/NERSC 2014 – 2019

ASCR Leadership Computing Challenge Award (175M CPU Hours, Co-PI), DOE/ALCF 2015

ASCR Leadership Computing Challenge Award (350M CPU Hours, Co-PI), DOE/ALCF 2014

PROFESSIONAL AFFILIATIONS

Review Editor: Frontiers in Physics, Frontiers in Chemistry 2022 – 2025
Member: American Chemical Society, American Physical Society, Materials Research Society

SCIENTIFIC SOFTWARE DEVELOPMENT

Quantum ESPRESSO: Active Developer/Co-Author 2012 – present

PUBLICATIONS

32. D. Ranabhat, P. Calvert, Y. Song, and **H.-Y. Ko***, *The High-Pressure Radical Chain-Growth Reaction Profile of Polyethylene Oligomers*, (in preparation).
31. T. Shah, Y. Song, A. Shastri, and **H.-Y. Ko***, *Can Different Orbital Localization Methods Account for Long-Range Electrostatics in Machine-Learning Force Fields?*, (in preparation).
30. B. K. Gunawardana, T. Shah, B. Azizova, D. Ranabhat, Y. Song, S. Ghose, A. Shastri, T. E. Gartner*, and **H.-Y. Ko***, *Structures of Polyethylene Oligomers During High-Pressure Radical Polymerization from Ab Initio Deep Potential Molecular Dynamics*, (in preparation).
29. **H.-Y. Ko***, M. F. Calegari Andrade, Z. M. Sparrow, B. G. Ernst, P. T. Lin, and R. A. DiStasio Jr.*, *Reactive Transport of Water Ions: Presolvated Proton Donors behind the Scenes*, (in preparation).
28. Z. M. Sparrow, **H.-Y. Ko**, J. Zhang, and R. A. DiStasio Jr., *Enabling Linear Scaling Exact Exchange for Heterogeneous Systems*, (in preparation).
27. S. Maiti, K. Dhakal, Y. Song, A. Kaffle, D. Ranabhat, L. Chen, **H.-Y. Ko***, A. K. Gupta, R. Roknuzzaman, G. Verma, K. Biradha, F. D'Souza*, T. AlShahrani, and S. Ma*, *Rational Design of Bimetallic 2D Covalent Organic Frameworks for Interlayer Electrocatalytic Urea Production from N₂ and CO₂*, Chem. Mater. **38**, 5566 (2026).
26. E. T. Ritz, G. Khalsa, **H.-Y. Ko**, R. A. DiStasio Jr., and N. A. Benedek, *Mechanical Properties of Solids from Maximally Localized Wannier Functions*, (in preparation), preprint: <https://arxiv.org/abs/2510.11945>.
25. S. Singh, M. Ghafariasl, **H.-Y. Ko**, S. Gamage, R. A. DiStasio Jr., M. Snure, Y. Abate, *Substrate Induced van der Waals Force Effect on the Stability of Violet Phosphorous*, Adv. Mater. Interfaces 2400326 (2024).
24. K. Li, **H.-Y. Ko**, R. A. DiStasio Jr., and A. Damle, *An unambiguous and robust formulation for Wannier localization*, Phys. Rev. B **110**, 085127 (2024).
23. **H.-Y. Ko**, M. F. Calegari Andrade, Z. M. Sparrow, J. Zhang, and R. A. DiStasio Jr., *High-Throughput Condensed-Phase Hybrid Density Functional Theory for Large-Scale Finite-Gap Systems: The *SeA* Approach*, J. Chem. Theory Comput. **19**, 4182 (2023).
22. Y. Yang, Y.-T. Shao, X. Lu, Y. Yang, **H.-Y. Ko**, R. A. DiStasio Jr., F. J. DiSalvo, D. A. Muller, and H. D. Abruña, *Elucidating Cathodic Corrosion Mechanisms with Operando Electrochemical Transmission Electron Microscopy*, J. Am. Chem. Soc. **144**, 15698 (2022).
21. Y. Yang, C. R. Peltier, R. Zeng, R. Schimmenti, Q. Li, X. Huang, Z. Yan, G. Potsi, R. Selhorst, X. Lu, W. Xu, M. Tader, A. V. Soudackov, H. Zhang, M. Krumov, E. Murray, P. Xu, J. Hitt, L. Xu, **H.-Y. Ko**, B. G. Ernst, C. Bundschu, A. Luo, D. Markovich, M. Hu, C. He, H. Wang, J. Fang, R. A. DiStasio Jr., L. F. Kourkoutis, A. Singer, K. J. T. Noonan, L. Xiao, L. Zhuang, B. S. Pivovar, P. Zelenay, E. Herrero, J. M. Feliu, J. Suntivich, E. P. Giannelis, S. Hammes-Schiffer, T. Arias, M. Mavrikakis, T. E. Mallouk, J. D. Brock, D. A. Muller, F. J. DiSalvo, G. W. Coates, and H. D. Abruña, *Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies*, Chem. Rev. **112**, 6117 (2022). **Cover Article**

20. **H.-Y. Ko**, B. Santra, and R. A. DiStasio Jr., *Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics II: Extensions to the Isobaric-Isoenthalpic and Isobaric-Isothermal Ensembles*, J. Chem. Theory Comput. **17**, 7789 (2021).
19. W. You, J. M. Ganley, B. G. Ernst, C. Peltier, **H.-Y. Ko**, R. A. DiStasio Jr., R. R. Knowles, and G. W. Coates, *Expeditious Synthesis of Aromatic-Free Piperidinium-Functionalized Polyethylene as Alkaline Anion Exchange Membranes*, Chem. Sci. **12**, 3898 (2021). **Chem. Sci. HOT Article**
18. C. Andreani, G. Romanelli, A. Parmentier, R. Senesi, A. I. Kolesnikov, **H.-Y. Ko**, M. F. Calegari Andrade, and R. Car, *Hydrogen Dynamics in Supercritical Water Probed by Neutron Scattering and Computer Simulations*, J. Phys. Chem. Lett. **11**, 9461 (2020).
17. **H.-Y. Ko**, J. Jia, B. Santra, X. Wu, R. Car, and R. A. DiStasio Jr., *Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics I: Theory, Algorithm, and Performance*, J. Chem. Theory Comput. **16**, 3757 (2020).
16. F. Tang, X. Jiang, **H.-Y. Ko**, J. Xu, M. Topsakal, G. Hao, A. T. N'Diaye, P. A. Dowben, D. Lu, X. Xu, and X. Wu, *Probe Ferroelectricity by X-ray Absorption Spectroscopy in Molecular Crystal*, Phys. Rev. Materials **4**, 034401 (2020).
15. T. Suh, Y. Yang, P. Zhao, K. U. Lao, **H.-Y. Ko**, J. Wang, R. A. DiStasio Jr., and J. Engstrom, *Competitive Adsorption as a Route to Area-Selective Deposition*, ACS Appl. Mater. Interfaces **12**, 9989 (2020).
14. M. F. Calegari Andrade, **H.-Y. Ko**, L. Zhang, R. Car, and A. Selloni, *Free Energy of Proton Transfer at the Water - TiO₂ Interface from Ab Initio Deep Potential Molecular Dynamics*, Chem. Sci. **11**, 2335 (2020).
13. **H.-Y. Ko**, L. Zhang, B. Santra, H. Wang, W. E, R. A. DiStasio Jr., and R. Car, *Isotope Effects in Liquid Water via Deep Potential Molecular Dynamics*, Mol. Phys. **117**, 3269 (2019). **Invited Article**
12. J. Hoja, **H.-Y. Ko**, M. A. Neumann, R. Car, R. A. DiStasio Jr., and A. Tkatchenko, *Reliable and Practical Computational Prediction of Molecular Crystal Polymorphs*, Science Adv. **5**, eaau3338 (2019).
11. M. F. Calegari. Andrade, **H.-Y. Ko**, R. Car, and A. Selloni, *Structure, Polarization, and Sum Frequency Generation Spectrum of Interfacial Water on Anatase TiO₂*, J. Phys. Chem. Lett. **9**, 6716 (2018).
10. B. Santra, **H.-Y. Ko**, Y. W. Yeh, F. Martelli, I. Kaganovich, Y. Raitses, and R. Car, *Root-Growth of Boron Nitride Nanotubes: Experiments and Ab Initio Simulations*, Nanoscale **10**, 22223 (2018). **Back Cover Article**
9. **H.-Y. Ko**, R. A. DiStasio Jr., B. Santra, and R. Car, *Thermal Expansion in Dispersion-Bound Molecular Crystals*, Phys. Rev. Materials **2**, 055603 (2018).
8. L. Zheng, M. Chen, Z. Sun, **H.-Y. Ko**, B. Santra, P. Dhuvad, and X. Wu, *Structural, Electronic, and Dynamical Properties of Liquid Water by Ab Initio Molecular Dynamics Based on SCAN Functional within the Canonical Ensemble*, J. Chem. Phys. **148**, 164505 (2018). **Editor's Pick**
7. M. Chen, L. Zheng, B. Santra, **H.-Y. Ko**, R. A. DiStasio Jr., M. L. Klein, R. Car, and X. Wu, *Hydroxide Diffuses Slower than Hydronium in Water Because its Solvated Structure Inhibits Correlated Proton Transfer*, Nat. Chem. **10**, 413 (2018).
6. F. Martelli, **H.-Y. Ko**, E. C. Oguz, and R. Car, *Local-Order Metric for Condensed-Phase Environments*, Phys. Rev. B **97**, 064105 (2018).
5. F. Martelli, **H.-Y. Ko**, C. C. Borallo, and G. Franzese, *Structural Properties of Water Confined by Phospholipid Membranes*, Front. Phys. **13**, 136801 (2018).

4. P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. B. Nardelli, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. Carnimeo, A. D. Corso, S. de Gironcoli, P. Delugas, R. A. DiStasio Jr., A. Ferretti, A. Floris, G. Fratesi, G. Fugallo, R. Gebauer, U. Gerstmann, F. Giustino, T. Gorni, J. Jia, M. Kawamura, **H.-Y. Ko**, A. Kokalj, E. Küçükbenli, M. Lazzeri, M. Marsili, N. Marzari, F. Mauri, N. L. Nguyen, H.-V. Nguyen, A. Otero-de-la-Roza, L. Paulatto, S. Poncé, D. Rocca, R. Sabatini, B. Santra, M. Schlipf, A. P. Seitsonen, A. Smogunov, I. Timrov, T. Thonhauser, P. Umari, N. Vast, X. Wu, and S. Baroni, *Advanced Capabilities for Materials Modelling with Quantum ESPRESSO*, J. Phys.: Condens. Matter **29**, 465901 (2017).
3. M. Chen, **H.-Y. Ko**, R. C. Remsing, M. F. Calegari Andrade, B. Santra, Z. Sun, A. Selloni, R. Car, M. L. Klein, J. P. Perdew, and X. Wu, *Ab Initio Theory and Modeling of Water*, Proc. Natl. Acad. Sci. USA **114**, 10846 (2017).
2. A. M. Reilly, R. I. Cooper, C. S. Adjiman, S. Bhattacharya, A. D. Boese, J. G. Brandenburg, P. J. Bygrave, R. Bylsma, J. E. Campbell, R. Car, D. H. Case, R. Chadha, J. C. Cole, K. Cosburn, H. M. Cuppen, F. Curtis, G. M. Day, R. A. DiStasio Jr., A. Dzyabchenko, B. P. van Eijck, D. M. Elking, J. A. van den Ende, J. C. Facelli, M. B. Ferraro, L. Fusti-Molnar, C.-A. Gatsiou, T. S. Gee, R. de Gelder, L. M. Ghiringhelli, H. Goto, S. Grimme, R. Guo, D. W. M. Hofmann, J. Hoja, R. K. Hylton, L. Iuzzolino, W. Jankiewicz, D. T. de Jong, J. Kendrick, N. J. J. de Klerk, **H.-Y. Ko**, L. N. Kuleshova, X. Li, S. Lohani, F. J. J. Leusen, A. M. Lund, J. Lv, Y. Ma, N. Marom, A. E. Masunov, P. McCabe, D. P. McMahon, H. Meekes, M. P. Metz, A. J. Misquitta, S. Mohamed, B. Monserrat, R. J. Needs, M. A. Neumann, J. Nyman, S. Obata, H. Oberhofer, A. R. Oganov, A. M. Orendt, G. I. Pagola, C. C. Pantelides, C. J. Pickard, R. Podeszwa, L. S. Price, S. L. Price, A. Pulido, M. G. Read, K. Reuter, E. Schneider, C. Schober, G. P. Shields, P. Singh, I. J. Sugden, K. Szalewicz, C. R. Taylor, A. Tkatchenko, M. E. Tuckerman, F. Vacarro, M. Vasileiadis, A. Vazquez-Mayagoitia, L. Vogt, Y. Wang, R. E. Watson, G. A. de Wijs, J. Yang, Q. Zhu, and C. R. Groom, *Report on the Sixth Blind Test of Organic Crystal Structure Prediction Methods*, Acta Crystallogr., Sect. B: Struct. Sci. **72**, 439 (2016).
1. Y. Shen, **H.-Y. Ko**, Q. Ai, S.-M. Peng, and B.-Y. Jin, *Molecular Split-Ring Resonators Based on Metal String Complexes*, J. Phys. Chem. C **118**, 3766 (2014).

INVITED PRESENTATIONS

15. “Towards a Non-Empirical Prediction of Condensed-Phase Polymer Structures: Deep Potential Molecular Dynamics Trained with Hybrid Density Functional Theory”, *Oral*, Chemistry and Biochemistry Seminar, Texas Woman’s University (2025).
14. “High-Throughput Hybrid DFT for Large-Scale Condensed-Phase Systems Using SeA”, *Oral*, Materials Science and Engineering Graduate Seminar, UNT (2025).
13. “High-Throughput Hybrid DFT for Large-Scale Condensed-Phase Systems Using SeA”, *Oral*, Mathematical Sciences Colloquium, Rensselaer Polytechnic Institute (2025).
12. “High-Throughput Hybrid DFT for Large-Scale Condensed-Phase Systems Using SeA”, *Oral*, Annabella Selloni Retirement Symposium, Princeton University (2025).
11. “High-Throughput Hybrid DFT for Complex Condensed-Phase Systems Containing Thousands of Atoms Using SeA”, *Oral*, “Can Ice Be Described from First Principles?” Symposium, The Centre for Advanced Study (CAS) at The Norwegian Academy of Science and Letters (2025).
10. “Reactive Grotthuss Transport of H_3O^+ and OH^- Through Aqueous Solutions: Proton Donors Behind the Scenes”, *Oral*, American Physical Society Global Physics Summit (2025).
9. “High-Throughput Hybrid Density Functional Theory for Complex Condensed-Phase Systems Containing Thousands of Atoms Using SeA”, *Oral*, Texas Computational Chemistry Symposium (2025).

8. "Towards an Accurate and Efficient First-Principles Description of Complex Condensed-Phase Systems: Structure, Stability, and Reactive Transport", *Oral*, Colorado School of Mines (2023).
7. "Towards an Accurate and Efficient First-Principles Description of Complex Condensed-Phase Systems: Structure, Stability, and Reactive Transport", *Oral*, University of North Texas (2023).
6. "Towards an Accurate and Efficient First-Principles Description of Complex Condensed-Phase Systems: Structure, Stability, and Reactive Transport", *Oral*, North Carolina State University (2023).
5. "Towards an Accurate and Efficient Order- N HPC Framework for Large-Scale Condensed-Phase Hybrid Density Functional Theory", *Oral*, NERSC Seminar Series (2021).
4. "Quantum ESPRESSO and GPU implementation of *Ab Initio* Molecular Dynamics (part II)", *Oral*, CSI Center Workshop (2019).
3. "Thermal Expansion in Dispersion-Bound Molecular Crystals", *Oral*, Cornell Theoretical Chemistry Journal Club (2019).
2. "Anharmonic Effects from Dispersion in Weakly Bound Molecular Crystals", *Poster*, Modeling Many-Body Interactions (MMBI15) Workshop (2015).
1. "A General Purpose Massively Parallel *Ab Initio* Molecular Dynamics Implementation with a Linear Scaling Exact Exchange Algorithm", *Poster*, PICSciE Workshop (2015).

CONTRIBUTED PRESENTATIONS

22. "Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based *Ab Initio* Molecular Dynamics: Application to the Ice Ih-II-III Triple Point", *Oral*, ACS Spring Meeting (2024).
21. "Expressway towards Heaven: High-Throughput Hybrid Density Functional Theory for Complex Condensed-Phase Systems Containing Thousands of Atoms Using **SeA**", *Poster*, ACS Spring Meeting (2024).
20. "Robust, Accurate, and Efficient Hybrid Density Functional Theory Framework for Large-Scale Condensed-Phase Systems", *Poster*, ACS Spring Meeting (2024).
19. "Fueling a Data-Driven Model for Confined $\text{H}_3\text{O}^+/\text{OH}^-$ Transport: A High-Throughput Framework for Condensed-Phase Hybrid DFT", *Oral*, APS March Meeting (2022).
18. "Accurate and Efficient Order- N Framework for Hybrid DFT Based *Ab Initio* Molecular Dynamics of Heterogeneous Finite-Gap Condensed-Phase Systems", *Poster & Sci-Mix*, ACS Fall Meeting (2021).
17. "Enabling Linear Scaling Exact Exchange for Heterogeneous Systems", *Oral*, APS March Meeting (2021).
16. "Improving the Scalability of Condensed-Phase Hybrid Density Functional Theory: Computation, Communication, and Load Balancing", *Oral*, APS March Meeting (2020).
15. "Quantum Effects in Condensed-Phase Systems", *Oral*, GPS Seminar of Department of Chemistry and Chemical Biology, Cornell University (2019).
14. "Enabling Large-Scale Isobaric-Isothermal Hybrid Density Functional Theory Simulations in the Condensed Phase", *Oral*, APS March Meeting (2019).
13. "Thermal Expansion of Dispersion-Bound Molecular Crystals", *Poster*, Princeton Chemistry Retreat (2018).
12. "A Hybrid Version of the SCAN Functional Including Long-Range Dispersion Interactions", *Oral*, APS March Meeting (2017).
11. "A Hybrid Version of the van der Waals Inclusive SCAN Functional", *Poster*, SCAN Workshop (2017).

10. “The Role of Anharmonicity and Nuclear Quantum Effects in the Pyridine Molecular Crystal: An *Ab Initio* Molecular Dynamics Study”, *Oral*, APS March Meeting (2016).
9. “Large-Scale Hybrid Density Functional Theory Calculations in the Condensed-Phase: *Ab Initio* Molecular Dynamics in the Isobaric-Isothermal Ensemble”, *Poster*, APS March Meeting (2016).
8. “Large-Scale *Ab Initio* Isobaric-Isothermal Simulations Using Self-Consistent van der Waals Inclusive Density Functionals”, *Poster*, PICSciE Workshop (2016).
7. “*Ab Initio* and Classical Simulations of the Condensed Phase Using High-Performance Computing”, *Poster*, ICTP Total Energy Meeting (2015).
6. “Large-Scale *Ab Initio* Isobaric-Isothermal Simulations Using Self-Consistent van der Waals Inclusive Density Functionals”, *Poster*, SciDAC (DOE) Meeting (2015).
5. “Large-Scale *Ab Initio* Isobaric-Isothermal Simulations Using Self-Consistent van der Waals Inclusive Density Functionals”, *Poster*, Princeton Chemistry Retreat (2015).
4. “van der Waals Interactions in Pyridine and Pyridine-Like Molecular Crystals: An *Ab Initio* Molecular Dynamics Study”, *Oral*, APS March Meeting (2014).
3. “All-In-One Scientific Research with SageTeX”, *Oral*, PyCon Taiwan (2012).
2. “Simple Analytical Expressions for the Persistent Current and Anapole Moment of Carbon Nanotori in the Thin Tubular Limit”, *Poster*, Annual Meeting of Chinese Chemical Society (2011).
1. “Theoretical Study of Quantum Particles Constrained on a D_{nh} Toroidal Surface—A Simple Free Electron Model for π -Electronic Structures of a Toroidal Carbon Nanotube”, *Poster*, National Taiwan University (2010).

PROFESSIONAL ACTIVITIES

Peer Reviewer (Academic Journals):

Nat. Comm.; J. Chem. Phys.; J. Phys.: Condens. Matter; Electron. Struct.; Front. Phys.; Front. Chem.; J. Appl. Phys.; Model. Simul. Mat. Sci. Eng.

Grant Review:

US Department of Energy (DOE), Office of Science SCGSR Program; American Chemical Society (ACS) Petroleum Research Fund (PRF); Swiss National Science Foundation (SNSF)

Professional Activities:

Member of 2026 Metropolis Dissertation Award Committee	2025
Co-Host of Prof. Adewumi Popoola’s USAfRI/APS Visit to Cornell University	2022
Co-Organizer of Science Communication Webinar, DOE BES ECN	2019
Co-Organizer of DOE BES ECN Meetup, APS March Meeting	2019
DOE BES ECN Representative of CSI Center, Princeton University	2018–2019
Volunteer for Morrel Cohen Symposium, Princeton University	2017
Co-Organizer of Chemistry Student-Invited Lecture Series (SILS), Princeton University	2017
Invited Attendee of Advanced Quantum ESPRESSO Developers’ Training Workshop, ICTP	2015

Mentoring at University of North Texas (UNT):

- Postdoctoral Research Associate

– Dr. Yizhi Song

2025/08–present

- Graduate Students
 - Kriti Alam 2025/10–present
 - Priya N. Limbu (co-advised with Prof. Mohammad Omary) 2025/07–present
 - Deepa Ranabhat 2024/11–present
 - Teresa Shah 2024/11–present
 - Bharatha K. Gunawardana 2024/01–present
- Undergraduate Students
 - Stacie Moreno (NSF REU) 2026/05–2026/07
 - Zoe Lindsey 2026/03–present
 - Juliana Trejo 2025/12–present
 - Peyton Calvert 2025/11–2026/05
 - Idil Tasyumruk 2025/08–2026/05
- High-School Students via The Texas Academy of Mathematics and Science (TAMS) Program
 - Anvitha Pasam 2025–present
 - Akshath Shastri 2024–present
 - Krish Kohir 2024–2025
 - Srinjoy Ghose 2024–2025

Mentoring Prior to UNT:

Mentor for undergraduate research, Cornell University	2024
Mentor for undergraduate research, Cornell University	2020 – 2021
Co-Mentor for Catalyzing Diversity in Chemistry Leadership, Princeton University	2014 & 2016
Co-Mentor for The Girls’ Science, Technology, Engineering, and Mathematics (GSTEM) summer research program, NYU Courant Institute of Mathematical Sciences	2014
Student Lecturer, Quasicrystal Conference, National Taiwan University	2012
Lecturer for elementary school students, National Taiwan Science Education Center	2012
Organizer and Demonstrator for the general public, Molecular Beading Exhibition, Taipei	2011
Lecturer (molecular structure) for high school students, National Taiwan University	2011
Lecturer (chemical kinetics) for high school students, National Taiwan University Chemistry Camp	2009