

YANG YANG

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Professional Profile

Assistant Professor **2019.08 – present**
Department of Chemistry, University of Wisconsin–Madison

Education and Training

Postdoctoral Associate **2016.08 – 2019.07**
University of Illinois at Urbana-Champaign and Yale University
Postdoctoral advisor: Sharon Hammes-Schiffer

Ph.D. Chemistry, Duke University **2011.08 – 2016.07**
Graduate advisor: Weitao Yang

B.S. Chemistry and Physics, Peking University **2007.09 – 2011.07**
Undergraduate advisor: Hong Jiang

Publications

At UW-Madison

- [1] Zehua Chen and **Yang Yang***, “The Constrained Nuclear-Electronic Orbital (CNEO) Framework for Nuclear Quantum Effects in Quantum Chemistry and Molecular Simulations”, Under revision
- [2] Haoran Chen, Yuzhe Zhang, Yiwen Wang, Kecai Xuan, Zehua Chen, and **Yang Yang***, “Analytic polarizability and vibrational Raman spectra from constrained nuclear-electronic orbital density functional theory”. *J. Chem. Phys.*, **163**, 244111 (2025)
- [3] Zhe Liu, Yiwen Wang, Yuzhe Zhang, Nan Yang, and **Yang Yang***, “Characterizing infrared spectra of $\text{OH}\cdot(\text{H}_2\text{O})_2$ and $\text{OH}\cdot(\text{H}_2\text{O})_3$ with constrained nuclear-electronic orbital molecular dynamics”. *J. Phys. Chem. A*, **129**, 9883 (2025)
- [4] Zehua Chen*, and **Yang Yang***, “Periodic constrained nuclear-electronic orbital

- density functional theory for nuclear quantum effects: Method development and application to hydrogen adsorption on Pt(111)". *J. Chem. Theory Comput.* **21**, 7865 (2025)
- [5] Tanner Culpitt*, Zehua Chen, Fabijan Pavošević, and **Yang Yang***, "Constrained nuclear-electronic orbital theory for quantum computation". *J. Chem. Theory Comput.* **21**, 7845 (2025)
- [6] Zhe Liu, Zehua Chen, and **Yang Yang***, "Nonadiabatic dynamics with constrained nuclear-electronic orbital theory". *J. Phys. Chem. Lett.* **16**, 6559 (2025)
- [7] Yuzhe Zhang, Zhe Liu, and **Yang Yang***, "Finite-temperature double proton transfer in formic acid dimer via constrained nuclear-electronic orbital molecular dynamics: Lower barriers and enhanced rates from nuclear quantum delocalization". *J. Chem. Theory Comput.* **21**, 5400 (2025)
- [8] Zehua Chen, Jingjing Zheng, Donald G. Truhlar, and **Yang Yang***, "Constrained nuclear-electronic orbital transition state theory using energy surfaces with nuclear quantum effects". *J. Chem. Theory Comput.* **21**, 590 (2025)
- [9] Jin Zhao, Zehua Chen, Zhihui Chen, Zeyi Meng, Jianwei Zhang, Wenjie Lv, Congshan Guo, Zhizhen Lv, Shouce Huang, **Yang Yang***, Zhongfan Liu*, Jingshu Hui*, "Epitaxy orientation and kinetics diagnosis for zinc electrodeposition", *ACS Nano* **19**, 736 (2025)
- [10] Yuzhuo Yang, Yuzhe Zhang, **Yang Yang***, and Xi Xu*, "Assessment of electron-proton correlation functionals for vibrational spectra of shared-proton systems by constrained nuclear-electronic orbital density functional theory", *J. Chem. Phys.* **161**, 244103 (2024)
- [11] Xianyuan Zhao, Zehua Chen, and **Yang Yang***, "Constrained nuclear-electronic orbital QM/MM approach for simulating complex systems with quantum nuclear delocalization effects incorporated", *Chem. Phys. Rev.* **5**, 041401 (2024) **Featured Article**
- [12] James Langford, Yuzhe Zhang, Zehua Chen, and **Yang Yang***, "Where is the hidden intramolecular H-bonding vibrational signal in proline?" *J. Chem. Phys.* **161**, 134302 (2024)
- [13] Kenneth D. Wilson, William H. Styers, Samuel A. Wood, R. Claude Woods, Robert J. McMahon, Zhe Liu, **Yang Yang**, and Etienne Garand*, "Spectroscopic quantification of the inverted singlet–triplet gap in pentaazaphenalene", *J. Am. Chem. Soc.* **146**, 15688 (2024)
- [14] Yuzhe Zhang, Yiwen Wang, Xi Xu, Zehua Chen, and **Yang Yang***, "Vibrational spectra of highly anharmonic water clusters: Molecular dynamics and harmonic analysis revisited with constrained nuclear-electronic orbital methods". *J. Chem. Theory Comput.* **19**, 9358 (2023)
- [15] Yuzhe Zhang, Xi Xu, Nan Yang, Zehua Chen, and **Yang Yang***, "Describing proton transfer modes in shared proton systems with constrained nuclear-electronic orbital methods", *J. Chem. Phys.* **158**, 231101 (2023) **Editor's pick, and part of the 2023 JCP Emerging Investigators Special Collection**

- [16] Yiwen Wang, Zehua Chen, and **Yang Yang**^{*}, “Calculating vibrational excited state absorptions with excited state constrained minimized energy surfaces”. *J. Phys. Chem. A*, **127**, 5491 (2023) *Published as part of The Journal of Physical Chemistry virtual special issue “Early-Career and Emerging Researchers in Physical Chemistry Volume 2”*
- [17] Yueqing Wang, Mingjie Chen, **Yang Yang**, John Ralph, and Xuejun Pan^{*}, “Efficient O-demethylation of lignin-derived aromatic compounds under moderate conditions”, *RSC Advances*, **13**, 5925 (2023)
- [18] Zehua Chen, and **Yang Yang**^{*}, “Incorporating nuclear quantum effects in molecular dynamics with a constrained minimized energy surface”, *J. Phys. Chem. Lett.* **14**, 279 (2023)
- [19] Xi Xu, Zehua Chen, and **Yang Yang**^{*}, “Molecular dynamics with constrained nuclear electronic orbital density functional theory: Accurate vibrational spectra from efficient incorporation of nuclear quantum effects”, *J. Am. Chem. Soc.* **144**, 4039 (2022)
- [20] James Langford, Xi Xu, and **Yang Yang**^{*}, “Plasmon character index: An accurate and efficient metric for identifying and quantifying plasmons in molecules”, *J. Phys. Chem. Lett.* **12**, 9391 (2021)
- [21] Xi Xu, and **Yang Yang**^{*}, “Molecular vibrational frequencies from analytic Hessian of constrained nuclear-electronic orbital density functional theory”, *J. Chem. Phys.* **154**, 244110 (2021), *part of 2021 JCP Emerging Investigator Special Collection*
- [22] Xi Xu, and **Yang Yang**^{*}, “Full-quantum descriptions of molecular systems from constrained nuclear-electronic orbital density functional theory”, *J. Chem. Phys.* **153**, 074106 (2020)
- [23] Xi Xu, and **Yang Yang**^{*}, “Constrained nuclear-electronic orbital density functional theory: Energy surfaces with nuclear quantum effects”, *J. Chem. Phys.* **152**, 084107 (2020)

Before UW-Madison

- [24] Tanner Culpitt, **Yang Yang**, Patrick E. Schneider, Fabijan Pavošević, and Sharon Hammes-Schiffer, “Molecular vibrational frequencies with multiple quantum protons within the nuclear-electronic orbital Framework”, *J. Chem. Theory Comput.* **15**, 6840 (2019)
- [25] Zhen Tao, **Yang Yang**, and Sharon Hammes-Schiffer, “Multicomponent density functional theory: Including the density gradient in the electron-proton correlation functional for hydrogen and deuterium”, *J. Chem. Phys.* **151**, 124102 (2019)
- [26] Tanner Culpitt, **Yang Yang**, Fabijan Pavošević, Zhen Tao, and Sharon Hammes-Schiffer, “Enhancing the applicability of multicomponent time-dependent density functional theory”, *J. Chem. Phys.* **150**, 201101 (2019)
- [27] **Yang Yang**, Patrick E. Schneider, Tanner Culpitt, Fabijan Pavošević, and Sharon

- Hammes-Schiffer, "Molecular vibrational frequencies within the nuclear–electronic orbital framework", *J. Phys. Chem. Lett.* **10**, 1167 (2019)
- [28] **Yang Yang**, Tanner Culpitt, Zhen Tao, and Sharon Hammes-Schiffer, "Stability conditions and local minima in multicomponent Hartree-Fock and density functional theory", *J. Chem. Phys.* **149**, 084105 (2018)
- [29] **Yang Yang**, Tanner Culpitt, and Sharon Hammes-Schiffer, "Multicomponent time-dependent density functional theory: Proton and electron excitation energies", *J. Phys. Chem. Lett.*, **9**, 1765 (2018)
- [30] Kurt R. Brorsen, **Yang Yang**, and Sharon Hammes-Schiffer, "Multicomponent density functional theory: Impact of nuclear quantum effects on proton affinities and geometries", *J. Phys. Chem. Lett.*, **8**, 3488 (2017)
- [31] **Yang Yang**, Kurt R. Brorsen, Tanner Culpitt, Michael V. Pak, and Sharon Hammes-Schiffer, "Development of a practical multicomponent density functional for electron-proton correlation to produce accurate proton densities", *J. Chem. Phys.* **147**, 114113 (2017)
- [32] Kurt R. Brorsen, **Yang Yang**, Michael V. Pak, and Sharon Hammes-Schiffer, "Is the accuracy of density functional theory for atomization energies and densities in bonding regions correlated?", *J. Phys. Chem. Lett.*, **8**, 2076 (2017)
- [33] Christopher Sutton, **Yang Yang**, Du Zhang, and Weitao Yang, "Single, double electronic excitations and exciton effective conjugation lengths in π -conjugated systems", *J. Phys. Chem. Lett.*, **9**, 4029 (2018)
- [34] Ye Jin, **Yang Yang**, Du Zhang, Degao Peng, and Weitao Yang, "Excitation energies from particle-particle random phase approximation with accurate optimized effective potentials", *J. Chem. Phys.* **147**, 134105 (2017)
- [35] Zehua Chen, Du Zhang, Ye Jin, **Yang Yang**, Neil Qiang Su, and Weitao Yang, "Multireference density functional theory with generalized auxiliary systems for ground and excited states", *J. Phys. Chem. Lett.*, **8**, 4479 (2017)
- [36] **Yang Yang**, Adriel Dominguez, Du Zhang, Thomas Frauenheim, and Weitao Yang, "Charge transfer excitations from particle-particle random phase approximation — Opportunities and challenges arising from two-electron deficient systems", *J. Chem. Phys.* **146**, 124104 (2017)
- [37] **Yang Yang**, Ernest Davidson, and Weitao Yang, "Nature of ground and electronic excited states of higher acenes", *Proc. Natl. Acad. Sci.*, **13**, E5098 (2016)
- [38] **Yang Yang**, Lin Shen, Du Zhang, and Weitao Yang, "Conical intersections from particle-particle random phase and Tamm-Dancoff approximations", *J. Phys. Chem. Lett.*, **7**, 2407 (2016)
- [39] **Yang Yang**, Kieron Burke, and Weitao Yang, "Accurate atomic quantum defects from particle–particle random phase approximation", *Mol. Phys.*, **114**, 1189 (2016)
- [40] **Yang Yang**, Degao Peng, Ernest Davidson, and Weitao Yang, "Singlet-triplet energy gaps for diradicals from particle-particle random phase approximation", *J. Phys. Chem. A*, **119**, 4923 (2015)

- [41] Degao Peng, **Yang Yang**, Peng Zhang, and Weitao Yang, "Restricted second random phase approximations and Tamm-Dancoff approximations for electronic excitation energy calculations", *J. Chem. Phys.* **141**, 214104 (2014)
- [42] **Yang Yang**, Degao Peng, Jianfeng Lu, and Weitao Yang, "Excitation energies from particle-particle random phase approximation: Davidson algorithm and benchmark studies", *J. Chem. Phys.* **141**, 124104 (2014)
- [43] Neil Shenvi, Helen van Aggelen, **Yang Yang**, and Weitao Yang, "Tensor hypercontracted ppRPA: Reducing the cost of the particle-particle random phase approximation from $O(r^6)$ to $O(r^4)$ ", *J. Chem. Phys.* **141**, 024119 (2014)
- [44] Degao Peng, Helen van Aggelen, **Yang Yang**, and Weitao Yang, "Linear-response time-dependent density-functional theory with pairing fields", *J. Chem. Phys.* **140**, 18A522 (2014)
- [45] Helen van Aggelen, **Yang Yang**, and Weitao Yang, "Exchange-correlation energy from pairing matrix fluctuation and the particle-particle random phase approximation", *J. Chem. Phys.* **140**, 18A511 (2014)
- [46] **Yang Yang**, Helen van Aggelen, and Weitao Yang, "Double, Rydberg and charge transfer excitations from pairing matrix fluctuation and particle-particle random phase approximation", *J. Chem. Phys.* **139**, 224105 (2013)
- [47] Yachao Zhang, **Yang Yang** and Hong Jiang, "3d–4f magnetic interaction with density functional theory plus U approach: Local coulomb correlation and exchange pathways", *J. Phys. Chem. A* **117**, 13194 (2013)
- [48] **Yang Yang**, Helen van Aggelen, Stephan N. Steinmann, Degao Peng, and Weitao Yang, "Benchmark tests and spin adaptation for the particle-particle random phase approximation", *J. Chem. Phys.* **139**, 174110 (2013)
- [49] Neil Shenvi, Helen van Aggelen, **Yang Yang**, Weitao Yang, Christine Schwerdtfeger, and David Mazziotti, "The tensor hypercontracted parametric reduced density matrix algorithm: coupled-cluster accuracy with $O(r^4)$ scaling", *J. Chem. Phys.* **139**, 054110 (2013)
- [50] Helen van Aggelen, **Yang Yang**, and Weitao Yang, "Exchange-correlation energy from pairing matrix fluctuation and the particle-particle random phase approximation", *Phys. Rev. A* **88**, 030501 (2013)
- [51] Jian Peng, Kuo-Chun Tang, Kaitlin McLoughlin, **Yang Yang**, Danika Forgach, and Roseanne J. Sension, "Ultrafast excited-state dynamics and photolysis in base-off B12 coenzymes and analogues: Absence of the trans-nitrogenous ligand opens a channel for rapid nonradiative decay", *J. Phys. Chem. B* **114**, 12398 (2010)

Honors and Awards

- ACS OpenEye Cadence Molecular Sciences Outstanding Junior Faculty Award in Computational Chemistry (ACS Spring 2026)
- CAREER award, National Science Foundation (2022)

- Honored Instructor, UW-Madison (2022, 2023)
- Outstanding Doctoral Dissertation Award in Theoretical Chemistry, Chinese Chemical Society (2017)
- Finalists for the Justin Jankunas Doctoral Dissertation Award, American Physical Society (2017)
- Paul M. Gross Fellowship, Duke University (2013)
- Outstanding Graduate Award, Peking University (2011)
- First prize of Beijing area in National Mathematical Contest in Modeling (2010)
- Founder Scholarship (2009 – 2010)
- First prize of “Jiang Zehan Cup” Mathematical Contest in Modeling (2010)
- Merit Student, Peking University (2009)
- Second prize of Beijing College Students' Physics Contest (2008)
- Suzhou Industrial Park Scholarship (2007 – 2008)

Student/Postdoc Awards (National Level)

- **Hypatia Newton**: ACS Scholarship for Undergraduates in Chemistry (2025)
- **Yiwen Wang**: MolSSI Software Fellowship (2024)
- **Zehua Chen**: Young Investigator Awards in Physical Chemistry, ACS PHYS Division (2024)
- **Zehua Chen**: Wiley Computers in Chemistry Outstanding Postdoc Award, ACS COMP Division (2024)

Presentations

Scheduled

- Dynamic Processes in Electrolytes and Biomolecular Systems Symposium, ACS Fall 2026, Chicago, IL, 08/2026
- Marcus Center Workshop on Electronic Structure Theory, California Institute of Technology, CA, 06/2026
- International Congress of Quantum Chemistry (ICQC), Berkeley, CA, 06/2026
- OpenEye Cadence Molecular Sciences Outstanding Junior Faculty Award Symposium, ACS Spring 2026, Atlanta, GA, 03/2026
- New York University 03/2026

Past

- University of Wisconsin-Madison 12/2025
- University of California, San Diego 12/2025

- University of California, Irvine 12/2025
- Rutgers University-New Brunswick 10/2025
- Rutgers University-Newark 10/2025
- University of Illinois at Urbana-Champaign 10/2025
- Columbia University 10/2025
- Yale University 10/2025
- California Institute of Technology 10/2025
- Purdue University 10/2025
- University of North Carolina 09/2025
- Duke University 09/2025
- North Carolina State University 09/2025
- University of California, Berkeley 09/2025
- History of Quantum Chemistry Symposium, ACS Fall 2025, Washington, DC, 08/2025
- 55th Midwest Theoretical Chemistry Conference (MWTCC), Wayne State University, Detroit, MI, 05/2025
- Rochester University, 04/2025
- 65th Sanibel Symposium, 02/2025
- Vanderbilt University, 02/2025
- Pacific Northwest National Laboratory, 01/2025
- University of Washington, 01/2025
- Virginia Commonwealth University, 01/2025
- 2nd PySCF Conference, California Institute of Technology, Pasadena, 01/2025
- 11th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP 2024), Qingdao, 10/2024
- University of Minnesota Twin Cities, 09/2024
- Hydrogen Bonding Interactions and Dynamics: Advanced Experimental and Theoretical Methods Symposium, APS March meeting, Minneapolis, MN, 03/2024
- University of Missouri, 02/2024
- University of California, Merced, 10/2023
- University of Massachusetts Amherst, 09/2023
- TSRC workshop — Quantum Effects in Condensed-Phase Systems, Telluride, CO, 07/2023
- Wayne State University, 04/2023
- Massachusetts Institute of Technology, 04/2023
- Boston University, 04/2023
- University of Wisconsin-Madison, 11/2022
- Virtual International Seminar on Theoretical Advancements (VISTA), 10/2022
- Purdue University, Virtual Theoretical and Computational Seminar, 09/2022
- Quantum Chemistry: Current & Future Frontiers Symposium, ACS Fall 2022, Chicago,

IL, 08/2022

- American Conference on Theoretical Chemistry, Lake Tahoe, CA, 07/2022
- Gordon Research Conference on Molecular Interactions and Dynamics, Stonehill College, MA, 07/2022
- Midwest Theoretical Chemistry Conference, Ohio State University, Columbus, OH, 06/2022
- Density Functional Theory and Beyond, APS March Meeting, Chicago, IL, 03/2022
- Symposium: Electronic and Nuclear Structure Theory: Quantum Dynamics for Electronic Ground and Excited States, Virtual Pacificchem Conference, 12/2021

Before UW-Madison

- Gordon Research Conference on Computational Chemistry, Promoted talk from poster, Mount Snow, VT, 2018
- Solar meeting, Yale University, 2018
- American Physical Society March Meeting, Contributed talk, Baltimore, MD, 2016
- TSRC workshop — Excited States and Time-Dependent Electronic Structure Theory, Contributed talk, Telluride, CO, 2014
- American Physical Society March Meeting, Contributed talk, Denver, CO, 2014

Grants

- **U.S. Department of Energy — Scientific Discovery through Advanced Computing (SciDAC)**

Developing Advanced Methods for Nuclear Quantum Effects on Emergent Phenomena in Molecular and Condensed-Phase Systems; Co-PI. Total award: \$10,000,000; UW–Madison subaward (PI: Yang Yang): \$800,000.

- **National Science Foundation — Cyberinfrastructure for Sustained Scientific Innovation (CSSI)**

Elements: Cyberinfrastructure for Incorporating Nuclear Quantum Effects in ab initio Molecular Simulations via Constrained Nuclear–Electronic Orbital Density Functional Theory (CNEO-DFT); Principal Investigator (sole PI); \$600,000; 09/2024 – 08/2027.

- **National Science Foundation — CAREER Award**

Development of Constrained Multicomponent Density Functional Theory and Accurate, Efficient Incorporation of Nuclear Quantum Effects in ab initio Molecular Dynamics; Principal Investigator (sole PI); \$650,000; 12/2022 – 11/2027.

Teaching

CHEM 562: Physical Chemistry II (Undergraduate Quantum and Statistical Mechanics)	19F, 20F, 21F
CHEM 563/4: Physical Chemistry Lab 1/2 (Undergraduate)	26S
CHEM 960: Physical Chemistry Seminar (Graduate)	20S, 22S, 24S, 25S
CHEM 775: Electronic Structure of Molecules (Graduate)	21S, 23S, 24F
CHEM 103: General Chemistry I (Undergraduate)	22F, 23F

Service

Journal Review

Journal of Chemical Physics, Journal of Chemical Theory and Computation, Journal of Physical Chemistry, Physical Review, Journal of Computational Chemistry, Theoretical Chemistry Accounts, Computational and Theoretical Chemistry, Chemical Physics, Chemical Physics Letters, Computer Physics Communications, Journal of the American Chemical Society, Nature Communications

Grant Review

- National Science Foundation (2022, 2023)
- U.S. Department of Energy (2022, 2023, 2026)
- American Chemical Society Petroleum Research (2023, 2025, 2026)
- Swiss National Science Foundation (2025)

Conference Organization

- **Electronic Structure Workshop** — Co-organizer (with Yuan Ping, J. R. Schmidt, Matthew Otten, Elio Koenig-Tarasevich, Ilya Esterlis); University of Wisconsin–Madison, Madison, WI (2026).
- **Symposium in Honor of the 65th Birthday of Dr. Weitao Yang: DFT and Beyond** — Lead organizer (with G. Andrés Cisneros and Paul Ayers); ACS Spring Meeting, Atlanta, GA (2026).
- **Focus Topic: Density Functional Theory in Chemical Physics** — Co-organizer (with Weitao Yang); APS Global Physics Summit, Anaheim, CA (2025).
- **54th Midwest Theoretical Chemistry Conference** — Lead organizer; Madison, WI (May 30–June 1, 2024).
- **Symposium: Recent Progress in Theoretical Methods for Coupled Quantum Systems** — Co-organizer (with Kurt Brorsen and Sharon Hammes-Schiffer); ACS Spring Meeting, New Orleans, LA (2024).

Other Professional Activities

- **Editorial Advisory Board Member**, *The Journal of Chemical Physics* — 01/2024–12/2025.
- **Panelist** (post-secondary instructor representative), Wisconsin Society of Science Teachers (WSST) Conference — 04/2024.

Students and Postdocs Supervised

Graduate Students (current)

- | | |
|---------------|-------------------|
| • Zhe Liu | 12/2021 – present |
| • Yiwen Wang | 12/2022 – present |
| • Yuzhe Zhang | 12/2022 – present |
| • Haoran Chen | 12/2024 – present |
| • Lin Han | 02/2025 – present |

Postdoctoral Associates (current)

- | | |
|---------------------|-------------------|
| • Dr. Zehua Chen | 06/2021 – present |
| • Dr. Xianyuan Zhao | 03/2023 – present |

Undergraduate Students (current)

- | | |
|------------------|-------------------|
| • Hypatia Newton | 01/2025 – present |
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Graduate Alumni

- | | |
|----------------------|-------------------|
| • Dr. James Langford | 12/2019 – 08/2024 |
|----------------------|-------------------|

Postdoctoral Alumni

- | | |
|---|-------------------|
| • Dr. Xi Xu | 09/2019 – 03/2022 |
| Current position: Assistant professor, Beijing Normal University, Zhuhai, China | |
| • Dr. Tanner Culpitt (Affiliated Hirschfelder Postdoc) | 09/2023 – 09/2025 |
| Current position: Research Scientist, University of Washington, Seattle, WA | |