YANG YANG

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University of Wisconsin–Madison
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EDUCATION

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

B.S. Chemistry, Peking University **2007.09 – 2011.07**
B.S. Physics, Peking University **2009.09 – 2011.07**
Undergraduate advisor: Hong Jiang

PROFESSIONAL EXPERIENCE

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

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

PUBLICATIONS

At UW-Madison

Submitted (Available through ChemRxiv)

[1] Zehua Chen, Jingjing Zheng, Donald G. Truhlar, and **Yang Yang***, "Constrained nuclear-electronic orbital transition state theory using energy surfaces with nuclear quantum effects". https://doi.org/10.26434/chemrxiv-2024-9q0hj-v2

Published

[2] 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**, 4, 041401 (2024) ***Editor's pick***

[3] 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)

[4] 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)

[5] 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)

[6] 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*

[7] 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"*

[8] 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)

[9] 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)

[10] 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)

[11] 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)

[12] 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*

[13] 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)

[14] 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

[15] 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)

[16] 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)

[17] 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)

[18] **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)

[19] **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)

[20] **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)

[21] 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)

[22] **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)

[23] 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)

[24] 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)

[25] 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)

[26] 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)

[27] **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)

[28] **Yang Yang**, Ernest Davidson, and Weitao Yang, “Nature of ground and electronic excited states of higher acenes”, *Proc. Natl. Acad. Sci.*, **13**, E5098 (2016)

[29] **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)

[30] **Yang Yang**, Kieron Burke, and Weitao Yang, "Accurate atomic quantum defects from particle–particle random phase approximation", *Mol. Phys.*, **114**, 1189 (2016)

[31] **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)

[32] 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)

[33] **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)

[34] 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)

[35] 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)

[36] 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)

[37] **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)

[38] 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)

[39] **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)

[40] 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)

[41] 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)

[42] 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

- 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)

NATIONAL LEVEL STUDENT/POSTDOC AWARDS

- Yiwen Wang: MolSSI Software Fellowship (2024)
- Dr. Zehua Chen: ACS PHYS Young Investigator Awards in Physical Chemistry (2024)
- Dr. Zehua Chen: Wiley Computers in Chemistry Outstanding Postdoc Award (2024)

PRESENTATIONS

Scheduled

1. Rochester University, 04/2025
2. 65th Sanibel Symposium, 02/2025
3. Vanderbilt University, 02/2025
4. University of Washington, 01/2025
5. 11th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP 2024), Qingdao, 10/2024

Past

6. University of Minnesota Twin Cities, 09/2024
7. Hydrogen Bonding Interactions and Dynamics: Advanced Experimental and Theoretical Methods, APS March meeting, 03/2024
8. University of Missouri, 02/2024
9. University of California, Merced, 10/2023

10. University of Massachusetts Amherst, 09/2023
11. TSRC workshop — Quantum Effects in Condensed-Phase Systems, Telluride, CO, 07/2023
12. Wayne State University, 04/2023
13. Massachusetts Institute of Technology, 04/2023
14. Boston University, 04/2023
15. University of Wisconsin-Madison, 11/2022
16. Virtual International Seminar on Theoretical Advancements (VISTA), 10/2022
17. Purdue University, Virtual Theoretical and Computational Seminar, 09/2022
18. American Chemical Society Fall Meeting, Quantum Chemistry: Current & Future Frontiers, Contributed talk, Chicago, IL, 08/2022
19. American Conference on Theoretical Chemistry, Promoted lightning talk, Lake Tahoe, CA, 07/2022
20. Gordon Research Conference on Molecular Interactions and Dynamics, Invited talk, Stonehill College, MA, 07/2022
21. Midwest Theoretical Chemistry Conference, Contributed talk, Ohio State University, Columbus, OH, 06/2022
22. American Physical Society March Meeting, Invited talk, Chicago, IL, 03/2022
23. Pacifichem, Contributed talk, Virtual, 12/2021
24. Gordon Research Conference on Computational Chemistry, promoted talk from poster, Mount Snow, VT, 2018
25. Solar meeting, Yale University, 2018
26. American Physical Society March Meeting, Contributed talk, Baltimore, MD, 2016
27. TSRC workshop — Excited States and Time-Dependent Electronic Structure Theory, Contributed talk, Telluride, CO, 2014
28. American Physical Society March Meeting, Contributed talk, Denver, CO, 2014

GRANTS

- National Science Foundation, *Elements: Cyberinfrastructure for incorporating nuclear quantum effects in ab initio molecular simulations through constrained nuclear-electronic orbital density functional theory*, $600,000, 2024/9-2027/8
- National Science Foundation CAREER award, *Development of Constrained Multicomponent Density Functional Theory and Accurate and Efficient Incorporation of Nuclear Quantum Effects in ab initio Molecular Dynamics*, $650,000, 2022/12-2027/11

TEACHING

CHEM562: Physical Chemistry II (Undergraduate Quantum and Statistical Mechanics) 19F, 20F, 21F

CHEM960: Physical Chemistry Seminar (Graduate) 20S, 22S, 24S

CHEM775: Electronic Structure of Molecules (Graduate) 21S, 23S, 24F
CHEM103: 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, Chemical Physics Letters, Computational and Theoretical Chemistry, Computer Physics Communications, Journal of the American Chemical Society, Nature Communications

Grant Review

- National Science Foundation (2022, 2023),
- Department of Energy (2022, 2023×2),
- American Chemical Society Petroleum Research Fund (2023)

Conference organization

Ongoing:

- Focus Topic: Density Functional Theory in Chemical Physics, co-organize with Weitao Yang, APS March meeting, Los Angeles, CA, 2025

Past:

- 54th Midwest Theoretical Chemistry Conference, Madison, 05/30/2024-06/01/2024
- Symposium: Recent Progress in Theoretical Methods for Coupled Quantum Systems, co-organize with Kurt Brorsen and Sharon Hammes-Schiffer, ACS Spring meeting, New Orleans, LA, 2024

Other

- Editorial Advisory Board, The Journal of Chemical Physics, 1/1/2024 – Present
- Panelist as representative of post-secondary instructors, Wisconsin Society of Science Teachers (WSST) Conference, 04/2024

STUDENTS AND POSTDOCS SUPERVISED

Current graduate students

- Zhe Liu 12/2021 – present
- Yiwen Wang 12/2022 – present
- Yuzhe Zhang 12/2022 – present

Current postdoctoral research assistants

- Zehua Chen 06/2021 – present
- Xianyuan Zhao 03/2023 – present
- Tanner Culpitt (Affiliated Hirschfelder Postdoc) 09/2023 – present

Former graduate student

- James Langford 12/2019 – 08/2024

Former postdoctoral research assistant

- Xi Xu 09/2019 – 03/2022
  Current position: Assistant professor, Beijing Normal University, Zhuhai, China