Yang Yang

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EDUCATION

Ph.D. Chemistry, Duke University **2011.08 – 2016.07**
Advisor: Prof. Weitao Yang
Thesis: Ground and Electronic Excited States from Pairing Matrix Fluctuation and Particle-Particle Random Phase Approximation

B.S. Chemistry, Peking University **2007.09 – 2011.07**
B.S. Physics, Peking University **2009.09 – 2011.07**
Advisor: Prof. Hong Jiang
Thesis: Theoretical Studies on 4f-3d Magnetic Interactions based on Density Functional Theory and Broken-Symmetry Approach

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
Advisor: Prof. Sharon Hammes-Schiffer

PUBLICATIONS

[1] 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.* Accepted (2019)

[2] 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)

[3] **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)

[4] **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)

[5] **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)

[6] 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)

[7] **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)

[8] 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)
[9] 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)
[10] 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)
[11] 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)
[12] **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)
[13] **Yang Yang**, Ernest Davidson, and Weitao Yang, "Nature of ground and electronic excited states of higher acenes", *Proc. Natl. Acad. Sci.*, **13**, E5098 (2016)
[14] **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)
[15] **Yang Yang**, Kieron Burke, and Weitao Yang, "Accurate atomic quantum defects from particle–particle random phase approximation", *Mol. Phys.*, **114**, 1189 (2016)
[16] **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)
[17] 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)
[18] **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)
[19] 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)
[20] 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)
[21] 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)
[22] **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)
[23] 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)
[24] **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)
[25] 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)
[26] 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)
[27] 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

- 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 Awards, 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)

CONFERENCE PRESENTATIONS

1. Selected talk from poster presentation, "Multicomponent Density Functional Theory and Time-Dependent Density Functional Theory Based on Nuclear-Electronic Orbital Approach", Gordon Research Conference on Computational Chemistry, Mount Snow, VT, 2018
2. Poster presentation, "Multicomponent Density Functional Theory and Time-Dependent Density Functional Theory Based on Nuclear-Electronic Orbital Approach", Gordon Research Conference on Computational Chemistry, Mount Snow, VT, 2018
3. Invited talk, "Multicomponent Density Functional Theory Based on Nuclear-Electronic Orbital Approach", Solar meeting, Yale University, 2018
4. Poster presentation "Development of a Practical Multicomponent Density Functional for Electron-Proton Correlation to Produce Accurate Proton Densities", American Conference on Theoretical Chemistry, Boston University, 2017.
5. Contributed talk, "Singlet-Triplet Energy Gaps for Diradicals from Particle-Particle Random Phase Approximation", Annual American Physical Society March Meeting, Baltimore, MD, 2016.
6. Contributed talk, "Excitation Energies from Particle-Particle Random Phase Approximation: Davidson Algorithm and Benchmark Studies", TSRC workshop — Excited States and Time-Dependent Electronic Structure Theory, Telluride, CO, 2014.
7. Contributed talk, "Double, Rydberg and Charge Transfer Excitations from Pairing Matrix Fluctuation and Particle-Particle Random Phase Approximation", Annual American Physical Society March Meeting, Denver, CO, 2014.
8. Poster presentation, "Ultrafast Transient Absorption Study of base-off Coenzyme B12", Summer Undergraduate Exchange Program, University of Notre Dame, 2009.

TEACHING

CHEM562 Physical Chemistry (II) **2019.09 – present**