Zehua Chen

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Education

August 2015–May 2021 — *Ph.D.* in Chemistry
Department of Chemistry
Duke University, Durham, NC, USA
Advisor: Weitao Yang

Sept. 2011–July 2015 — *Bachelor of Science* in Materials Chemistry
College of Chemistry and Molecular Engineering
Peking University, Beijing, PRC
Advisor: Hong Jiang

Professional Experience

June 2021–*Current* — *Research Associate*
Department of Chemistry
University of Wisconsin Madison, Madison, WI, USA
Advisor: Yang Yang

Publications

In preparation

(1) **Chen, Z.**, & Yang, Y. Constrained Nuclear-Electronic Orbital Full Configuration Interaction. In preparation.

(2) **Chen, Z.**, & Yang, Y. Constrained Nuclear-Electronic Orbital Density Functional Theory with Periodic Boundary Conditions: How Zero-Point Energy Affects Hydrogen Adsorption on Pt(111) Surface. In preparation.

Submitted

(3) **Chen, Z.**, Zheng, J., Truhlar, D. G., & Yang, Y. Transition State Theory within Constrained Nuclear-Electronic Orbital Framework: Accurate Hydrogen Atom Transfer Reaction Rates with Direct Incorporation of Quantum Nuclear Delocalization Effects. 10.26434/chemrxiv-2024-9q0hj, under second-round review with *Journal of the American Chemical Society*

(4) Yu, J., Mei, Y., **Chen, Z.**, & Yang, W. Accurate Prediction of Core Level Binding Energies from Ground-State Density Functional Calculations: The Importance of Localization and Screening. arXiv:2406.06345.

Published

(5) Zhao, X., **Chen, Z.**, & Yang, Y. Constrained Nuclear-Electronic Orbital QM/MM Approach for Simulating Complex Systems with Quantum Nuclear Delocalization Effects Incorporated. *Chemical Physics Reviews*, **2024**.

(6) Langford, J., Zhang, Y., **Chen, Z.**, & Yang, Y. Where is the Hidden Intramolecular H-bonding Vibrational Signal in the Proline Matrix IR Spectrum? *The Journal of Chemical Physics*, **2024**.

(7) **Chen, Z.**, & Yang, W. Development of a Machine Learning Finite-Range Nonlocal Density Functional. *The Journal of Chemical Physics*, **2024**, *160*(1), 014105.

(8) Zhang, Y., Wang, Y., Xu, X., **Chen, Z.**, & Yang, Y. Vibrational Spectra of Highly Anharmonic Water Clusters: Molecular Dynamics and Harmonic Analysis Revisited with Constrained Nuclear-Electronic Orbital Methods. *Journal of Chemical Theory and Computation*, **2023**, *19*(24), 9358-9368.

(9) Li, J., Yu, J., **Chen, Z.**, & Yang, W. Linear Scaling Calculations of Excitation Energies with Active-Space Particle-Particle Random-Phase Approximation. *The Journal of Physical Chemistry A*, **2023**, *127*(37), 7811-7822.

(10) Zhang, Y., Xu, X., Yang, N., **Chen, Z.**, & Yang, Y. Describing Proton Transfer Modes in Shared Proton Systems with Constrained Nuclear-Electronic Orbital Methods. *The Journal of Chemical Physics*, **2023**, *158*(23), 231101.

(11) Wang, Y., **Chen, Z.**, & Yang, Y. Calculating Vibrational Excited State Absorptions with Excited State Constrained Minimized Energy Surfaces. *The Journal of Physical Chemistry A*, **2023**, *127*(25), 5491-5501.

(12) **Chen, Z.**, & Yang, Y. Incorporating Nuclear Quantum Effects in Molecular Dynamics with a Constrained Minimized Energy Surface. *The Journal of Physical Chemistry Letters*, **2023**, *14*(1), 279-286.

(13) Xu, X., **Chen, Z.**, & Yang, Y. Molecular Dynamics with Constrained Nuclear Electronic Orbital Density Functional Theory: Accurate Vibrational Spectra from Efficient Incorporation of Nuclear Quantum Effects. *Journal of the American Chemical Society*, **2022**, *144*(9), 4039-4046.

(14) Mei, Y., Yu, J., **Chen, Z.**, Su, N. Q., & Yang, W. LibSC: Library for Scaling Correction Methods in Density Functional Theory. *The Journal of Chemical Theory and Computation*, **2022**, *18*(2), 840-850.

(15) Li, J., **Chen, Z.**, & Yang, W. Multireference Density Functional Theory for Describing Ground and Excited States with Renormalized Singles. *The Journal of Physical Chemistry Letters*, **2022**, *13*(3), 894-903.

(16) Mei, Y., **Chen, Z.**†, & Yang, W. Exact Second-Order Corrections and Accurate Quasiparticle Energy Calculations in Density Functional Theory. *The Journal of Physical Chemistry Letters*, **2021**, *12*(30), 7236-7244.

(17) Li, J., **Chen, Z.**, & Yang, W. Renormalized Singles Green's Function in the T-Matrix Approximation for Accurate Quasiparticle Energy Calculation. *The Journal of Physical Chemistry Letters*, **2021**, *12*(26), 6203-6210.

(18) Mei, Y., **Chen, Z.**†, & Yang, W. Self-Consistent Calculation of the Localized Orbital Scaling Correction for Correct Electron Densities and Energy-Level Alignments in Density Functional Theory. *The Journal of Physical Chemistry Letters*, **2020**, *11*(23), 10269-10277.

(19) Jin, Y., Su, N. Q., **Chen, Z.**, & Yang, W. Introductory Lecture: When the Density of the Noninteracting Reference System Is Not the Density of the Physical System in Density Functional Theory. *Faraday Discussions*, **2020**, *224*, 9-26.

(20) Li, G., **Chen, Z.**, Li, Y., Zhang, D., Yang, W., Liu, Y., & Cao, L. Engineering Substrate Interaction to Improve Hydrogen Evolution Catalysis of Monolayer MoS_2 Films Beyond Pt. *ACS nano*, **2020**, *14*(2), 1707-1714.

(21) Pinter, B., Al-Saadon, R., **Chen, Z.**, & Yang, W. Spin-State Energetics of Iron (II) Porphyrin from the Particle-Particle Random Phase Approximation. *The European Physical Journal B*, **2018**, *91*(11), 1-10.

(22) Jin, Y., Zhang, D., **Chen, Z.**, Su, N. Q., & Yang, W. Generalized Optimized Effective Potential for Orbital Functionals and Self-Consistent Calculation of Random Phase Approximations. *The Journal of Physical Chemistry Letters*, **2017**, *8*(19), 4746-4751.

(23) **Chen, Z.**, Zhang, D., Jin, Y., Yang, Y., Su, N. Q., & Yang, W. Multireference Density Functional Theory with Generalized Auxiliary Systems for Ground and Excited States. *The Journal of Physical Chemistry Letters*, **2017**, *8*(18), 4479-4485.

(24) Wang, Y. C., **Chen, Z. H.**, & Jiang, H. The Local Projection in the Density Functional Theory Plus U Approach: A Critical Assessment. *The Journal of Chemical Physics*, **2016**, *144*(14), 144106.

† indicates co-first authorship.

Honors and Awards

2024	Young Investigator Postdoc Award, ACS PHYS
2024	Wiley Computers in Chemistry Outstanding Postdoc Award, ACS COMP
2019	Kathleen Zielik Fellowship, Duke University
2014	Dow Scholarship, Peking University
2013	GuangHua Scholarship, Peking University
2012	Sumitomo Scholarship, Peking University

Presentations

ACS 2024 PHYS Award Talk	*Constrained Nuclear-Electronic Orbital (CNEO) Framework: Accurate and Efficient Incorporation of Nuclear Quantum Effects in Molecular Simulations and Reaction Kinetics*
ACS 2024 COMP Award Poster	*Constrained Nuclear-Electronic Orbital Transition State Theory Using Energy Surfaces with Nuclear Quantum Effects*
MWTCC 2024 Session Chair	*Electronic Structure*
MWTCC 2024 Poster	*Constrained Nuclear-Electronic Orbital Transition State Theory Using Energy Surfaces with Nuclear Quantum Effects*
APS 2024 Oral	*Transition State Theory within Constrained Nuclear-Electronic Orbital Framework: Accurate Adiabatic Hydrogen Atom Transfer Reaction Rates with Incorporation of Zero-Point Energy Effects*
MWTCC 2023 Oral	*Vibrations and Reactions by Constrained Nuclear-Electronic Orbital (CNEO) DFT: Nuclear Quantum Effects in Ab Initio Simulations*
ACTC 2022 Poster	*Incorporating Nuclear Quantum Effects in Molecular Dynamics*
APS 2022 Poster	*Incorporating Nuclear Quantum Effects in Molecular Dynamics*
ACS 2019 Oral	*Development of a Finite-Range Non-Local Functional, Assisted by Machine-Learning*

ACS 2018 Oral	*Multireference Density Functional Theory with Generalized Auxiliary Reference Systems for Ground and Excited States*
ACTC 2017 Poster	*Multireference Density Functional Theory with Generalized Auxiliary Reference Systems for Ground and Excited States*