XIAO WANG

PERSONAL INFORMATION

email	xwang89@vt.edu
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address	725 Independence Blvd, Christiansburg, VA USA

RESEARCH INTERESTS

Development of electronic structure theory with controlled accuracy and precision for prediction. Novel numerical representations for quantum mechanical treatment of large systems, especially condensed phase. High-performance implementation of quantum chemistry methods on modern massively parallel computer platforms.

EDUCATION

2012-2016 University of Georgia Athens, GA USA

Ph.D.

GPA: 3.7 · *Theoretical Chemistry*
Thesis title: *High Level Ab Initio Characterization of Small Hydrocarbons and Efficient Implementation of Density Cumulant Functional Theory*
Advisors: Prof. Henry F. Schaefer

2008-2012 Beihang University Beijing China

Bachelor of Science

GPA: 3.7 · *Applied Chemistry*

PROFESSIONAL EXPERIENCE

2016-2018 Virginia Tech

Postdoctoral Associate

- Developed the concentric atomic density fitting approach for the quantum mechanical exchange interaction in periodic systems, improving the efficiency relative to the conventional explicit method by an order of magnitude
- Implemented a massively-parallel periodic Hartree-Fock code from scratch in the MPQC package, using a block-sparse tensor library, TiledArray, and the task-based parallel runtime within MADNESS
- Incorporated a state-of-the-art resolution-of-the-identity algorithm and multipole approximation to further accelerate the computation of Coulomb interaction in periodic calculations

2014-2016 PSI4 Software Platform

Theory & Program Developer

- Derived working equations of a quantum chemistry method, DF-RDCT
- Implemented DF-RDCT equations in PSI4, interacting successfully with other functionalities in the PSI4 package
- Boosted the efficiency of original DCT by more than 10 times and applied it to transition metal compounds with up to 1000 basis functions

2012-2016 Center for Computational Quantum Chemistry

Leading Research Member

- Resolved the discrepancy between theory and experiment regarding the favored reaction path of cyclobutylidene, a nonclassical carbene involved in many reactions, with various *ab initio* methods
- Predicted and explained absorption/emission Near-IR spectra for an inorganic pigment, "Egyptian Blue", using Kohn-Sham DFT
- Predicted experimentally observable structures and fundamental frequencies of 90°-twisted triplet ethylene using coupled cluster theory along with VPT2

2015-2016 Center for Computational Quantum Chemistry

Research Mentor

- Guided junior graduate students through quantum chemistry theories and programs for predictions in organometallic chemistry projects
- Led undergraduate students to participate in a research team of eight in the study of various combustion chemistry processes

PUBLICATIONS

To Be Submitted

Sep. 2018 Efficient Parallel Implementation of Exact Exchange for Periodic Systems within Concentric Atomic Density Fitting Approximation

Authors: Xiao Wang and Edward F. Valeev

To Be Submitted

Sep. 2018 Intermediate Screening of Tensor Contractions in Concentric Atomic Density Fitting

Authors: Cannada A. Lewis, Xiao Wang, and Edward F. Valeev

Submitted to Energy Storage Mater.

Sep. 2018 Renewable-Lawsone-Based Sustainable and High-Voltage Aqueous Flow Battery

Authors: Pengfei Hu, Hao Lan, Xiao Wang, Yun Yang, Xiaoyu Liu, Hua Wang, Lin Guo

Org. Lett.

Nov. 2017 A Twist of the Twist Mechanism, 2-Iodoxybenzoic Acid (IBX)-Mediated Oxidation of Alcohol Revisited: Theory and Experiment

Authors: Heming Jiang, Tianyu Sun, Xiao Wang, Yaoming Xie, Xinhao Zhang, Yundong Wu, Henry F. Schaefer

Phys. Chem. Chem. Phys.

Aug. 2017 Radicals derived from acetaldehyde and vinyl alcohol

Authors: Marissa L. Estep, W. James Morgan, Alexander T. Winkles, Adam S. Abbott, Nery Villegas-Escobar, J. Wayne Mullinax, Walter E. Turner, Xiao Wang, Justin M. Turney and Henry F. Schaefer

J. Comput. Theory Chem.

May 2017 Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability

Authors: Robert M. Parrish, Lori A. Burns, Daniel G. A. Smith, Andrew C. Simmonett, A. Eugene DePrince, Edward G. Hohenstein, Uğur Bozkaya, Alexander Yu. Sokolov, Roberto Di Remigio, Ryan M. Richard, Jérôme F. Gonthier, Andrew M. James, Harley R. McAlexander, Ashutosh Kumar, Masaaki Saitow, Xiao Wang, Benjamin P. Pritchard, Prakash Verma, Henry F. Schaefer, Konrad Patkowski, Rollin A. King, Edward F. Valeev, Francesco A. Evangelista, Justin M. Turney , T. Daniel Crawford, and C. David Sherrill

J. Comput. Theory Chem.

June 2016 Spin-Adapted Formulation and Implementation of Density Cumulant Functional Theory with Density-Fitting Approximation: Application to Transition Metal Compounds

Authors: Xiao Wang, Alexander Y. Sokolov, Justin M. Turney, Henry F. Schaefer

Phys. Chem. Chem. Phys.

May 2016 Characterizing a Nonclassical Carbene with Coupled Cluster Methods: Cyclobutylidene

Authors: Xiao Wang, Jay Agarwal, Henry F. Schaefer

ChemPhysChem

Apr. 2016 1,1-Dilithioethylene: Toward Spectroscopic Identification of the Definitive Singlet Ground Electronic State of a Peculiar Structure

Authors: Yameng Liu, Xiao Wang, Yongdong Liu, Rugang Zhong, Yaoming Xie, Henry F. Schaefer

ChemComm — *Feb. 2016* Why Does Togni's Reagent I Exist in the High-Energy Hypervalent Iodine Form? Re-Evaluation of Benziodoxole Based Hypervalent Iodine Reagents

Authors: Tianyu Sun, Xiao Wang, Hao Geng, Yaoming Xie, Yundong Wu, Xinhao Zhang, Henry F. Schaefer

J. Phys. Chem. A — *Apr. 2014* Twisted Triplet Ethylene: Anharmonic Frequencies and Spectroscopic Parameters for C_2H_4, C_2D_4, and $^{13}C_2H_4$

Authors: Xiao Wang, Walter E. Turner, Jay Agarwal, Henry F. Schaefer

Analyst — *June 2012* Functionalized Gold Nanoparticles as Nanosensor for Sensitive and Selective Detection of Silver Ions and Silver Nanoparticles by Surface-Enhanced Raman Scattering

Authors: Enzhong Tan, Penggang Yin, Xiufeng Lang, Xiao Wang, Tingting You, Lin Guo

COMPUTER SKILLS

Basic — C++, Python, Fortran, LaTeX

Mathematical — Mathematica, Matlab

Computational — MPQC, Psi4, PySCF, Crystal, Cfour, Orca, Gaussian, Q-Chem, Molpro

OTHER INFORMATION

Presentations in Conferences

2018 · 30th Annual Workshop on Recent Developments in Electronic Structure Methods & Penn Conference in Theoretical Chemistry '18 in Philadelphia, PA

2017 · 11th Triennial Congress of the World Association of Theoretical and Computational Chemists in Munich, Germany

2016 · 56th Sanibel Symposium in St. Simons Island, GA

2015 · 250th American Chemical Association National Meeting in Boston, MA

2013 · 44th Southeastern Theoretical Chemistry Association Meeting in Auburn, AL

Interests — Tennis · Sci-Fi · Running

October 8, 2018