Yudong Qiu

Center for Computational Quantum Chemistry
Department of Chemistry
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EDUCATION

The University of Georgia — Athens, GA
PhD, Physical Chemistry — May 2015
Dissertation: "Pushing the Ab Initio Limits for the Accurate Characterization of Small Molecular Systems"
Committee: Profs. Henry F. Schaefer, Gary Douberly, Jeffery Urbauer

Nanjing University — Nanjing, China
BS, Chemistry — June 2011
Thesis: "Interactions of Polymer Adsorbed Between Thin Films"
Advisor: Prof. Rong Wang

RESEARCH EXPERIENCE

University of Georgia — Athens, GA
Research Assistant; Advisor: Prof. Henry F. Schaefer — 2011—Present
Computed properties for various systems

- Ground states, excited states, transition states for single- and multi-reference systems
- Energetics, structures, anharmonic vibrational frequencies, intrinsic reaction pathways, thermal reaction rates

Programmed Ab Initio methods

- MP2, CCSD, CCSD(T) using UHF reference and spin-adapted MP2, CCSD using RHF reference, with DIIS convergence acceleration method
- Spacial symmetry adopted using DPD method
- MP2-R12

Created Python scripts to automatically perform computations and analyze results

- Numerical displacements generated to obtain cubit and quartic force constants used in VPT2 theory
- Multi-dimensional scan of the potential energy surface
- Auto-generation and refinement of intrinsic reaction paths, with gradient and hessian information.

PUBLICATIONS

Y. Qiu, C. Wu, W. Allen, H. F. Schaefer and J. Agarwal, "σ Bond Activation Through Tunneling: Formation of the Boron Hydride Cations BH+n (n = 2, 4, 6) ". Submitted to *Phys. Chem. Chem. Phys.*

Y. Qiu, A. Y. Sokolov, Y. Yamaguchi and H. F. Schaefer, "$BeCH_2$: The Simplest Metal Carbene. High Levels of Theory" *J. Phys. Chem. A,* 2013, **117**, 9266-9273

H. Wang, **Y. Qiu**, H. F. Schaefer, "Pathways for the OH + Br_2 → HOBr + Br and HOBr + Br → HBr + BrO Reactions" Submitted to *J. Phys. Chem. A*.

H. Wang, **Y. Qiu**, G. Czako, H. F. Schaefer, "Reaction Pathways for OH + Cl_2 → HOCl + Cl → HCl + ClO" *J. Phys. Chem. A,* 2015, **119**, 7802-7809

Z. Jiang, C. Xu, **Y. Qiu**, X. Wang, D. Zhou, G. Xue, "Complex microstructures of ABC triblock copolymer thin films directed by polymer brushes based on self-consistent field theory", *Nanoscale Res. Lett.* 2014, **9**(1), 359

R. Wang, S. Zhang, **Y. Qiu**, "Hetero-structure of ABC triblock copolymer thin film on polymer-coated substrate" *Polymer*, 2011, **52**(2), 586-592

PRESENTATIONS

Y. Qiu, "Towards Quantum Chemistry on a Quantum Computer". Oral presentation at CCQC literature group meeting, 2014
Y. Qiu, "The Formation of BH_6^+ Characterized at the Ab Initio Limit". Poster presentation delivered at SETCA meeting held at Emory University, 2014
Y. Qiu, "Equation-of-Motion Coupled-Cluster Methods". Student lecture given in advanced quantum chemistry course, 2014
Y. Qiu, "An Introduction to the Domain-Based Local Pair Natural Orbital Coupled-cluster (DLPNO-CC) Methods". Oral presentation at CCQC group meeting, 2014
Y. Qiu, "Tensor Hypercontraction Density Fitting (THC-DF) Method". Oral presentation at CCQC literature group meeting, 2013
Y. Qiu, "Singlet and Triplet Potential Energy surface of $BeCH_2$". Poster presentation delivered at SETCA meeting held at University of Georgia, 2012

TEACHING EXPERIENCE

University of Georgia — Athens, GA
Teaching Assistant, General Chemistry — 2011—2012
Lecturer, CCQC Summer School — 2012—2014

- Lectures: Configuration Interaction, Perturbation Theory, Group Theory

SKILLS

Programming: C++/C, Python, Fortran, Objective-C, Swift
Quantum Chemistry Package: Psi4, CFOUR, Molpro, QChem, GAMESS, Polyrate
Software: Mathematica, Avogadro, ChemBioDraw, VMD, Adobe Photoshop and Illustrator, TeXShop(Latex)