

Jieyang GU

Bowling Green State University

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EDUCATION

Bowling Green State University, Bowling Green, Ohio, USA

Sep.2023 - Jul.2025

M.S. in Photochemical Sciences (GPA: 3.47/4)

- Major course: Quantum Chemistry, Photophysics etc.

East China Normal University (ECNU), Shanghai, China

Sep.2017 - Jul.2021

Physical Chemistry (*Incomplete due to personal health condition during COVID-19*)

- Major course: Quantum Chemistry, Statistical Thermodynamics, Computational Chemistry, Advanced Mathematics, etc.

Donghua University, Shanghai, China

Sep.2013 - Jul.2017

B.E. in Polymer Materials and Engineering (GPA: 2.46/4)

- Thesis: “*Preparation of Diamine Bisphosphine-Carbonyl-Iron (II) Complexes*” (Supervised by: Prof. Weiwei Zuo)
- Major course: Polymer Chemistry, Materials Science, Organic Chemistry, etc.

PUBLICATIONS

Jieyang Gu, Weiwei Zuo *. Non-Adiabatic Dynamic Simulation of the Decay Pathway of Oxopyrrolidine Switch Model Motor. (Under review in *Chemical Physics Letters*)

RESEARCH EXPERIENCES

1. Preparation of Diamine Bisphosphine-Carbonyl-Iron (II) Complexes.

- **Aim:** To synthesize and thoroughly characterize a series of diamine bisphosphine-carbonyl-iron (II) complexes, exploring their potential applications in coordination chemistry, such as catalysis and material science.
- **Method & Content:**
- Synthesis Process:** Designed a multi-step synthetic route for the preparation of the desired complexes. Utilized high-purity starting materials, including specific diamine and bisphosphine ligands, to ensure optimal reaction conditions. Controlled reaction parameters such as temperature, solvent choice, and reagent ratios to achieve efficient ligand coordination and iron complex formation. Isolated intermediates at each step and performed purification using techniques such as recrystallization and chromatography.
 - ¹H NMR Spectroscopy:** Conducted ¹H NMR analysis to determine the hydrogen environments in the synthesized intermediates and final complexes. Verified the ligand attachment and iron-ligand coordination by identifying chemical shifts and coupling constants specific to the complex structure.
 - ³¹P NMR Spectroscopy:** Applied ³¹P NMR spectroscopy to confirm the coordination of phosphine groups to the iron center. Monitored changes in the chemical environment of phosphorus atoms to ensure successful ligand integration.
 - Mass Spectrometry (MS):** Employed electrospray ionization (ESI-MS) and high-resolution mass spectrometry (HRMS) for molecular weight determination. Used fragmentation patterns to validate the molecular formula and connectivity within the complex.
- **Results:**
- Successfully synthesized diamine bisphosphine-carbonyl-iron (II) complexes.
 - Confirmed the molecular structure and composition through precise spectroscopic and mass spectrometric analysis.

2. Non-Adiabatic Dynamic Simulation of the Decay Pathway of Oxopyrrolidine Switch Model Motor.

- **Aim:** To investigate the non-adiabatic decay pathways of an oxopyrrolidine-based molecular switch to understand its photochemical mechanism and optimize its switching efficiency.
- **Method:**
 - a) **Dynamic Simulations:** Performed **trajectory simulations** using **Tully surface hopping** to model the evolution of the system under non-adiabatic conditions. Analyzed the transitions between excited states and ground states to capture the non-adiabatic dynamics.
 - b) **Conical Intersection Analysis:** Conducted **conical intersection optimizations** to identify critical regions where potential energy surfaces of electronic states intersect. Mapped out the **minimum energy pathways (MEP)** to trace the most probable decay routes.
 - c) **Computational Methods:** Utilized DFT (Density Functional Theory) for ground-state optimizations. Applied CASSCF (Complete Active Space Self-Consistent Field) to describe multi-reference wavefunctions for excited states. Performed high-accuracy energy calculations with CASPT2 (Complete Active Space with Perturbation Theory Level 2) to refine transition states and conical intersection energies.
 - d) **Software:** Gaussian was employed for initial structure optimizations and DFT calculations. Molcas was used for advanced multi-reference calculations and dynamic trajectory analysis.
- **Results:** Identified key decay pathways and conical intersections governing the switch mechanism.

3. Hartree-Fock Programming with Parallelized ERIs and Testing.

- **Aim:** To develop and optimize Hartree-Fock algorithms for improved computational efficiency in integral evaluations.
- **Method:**
 - a) **Algorithm Development:** Implemented parallelized ERI routines using advanced programming frameworks: C++: For core algorithm design and implementation of ERI evaluation. OpenMP: To enable multi-threaded parallelism on shared-memory architectures. MPI (Message Passing Interface): For distributing computations across multiple nodes in a cluster. CUDA: To offload computationally intensive tasks to GPUs for further acceleration. Applied mathematical optimizations, including analytical integral decomposition and symmetry exploitation, to reduce redundant calculations.
 - b) **Hardware and Software Environment:** Configured and built a custom Dell Precision T7810 workstation equipped with high-performance CPUs and NVIDIA GPUs to support algorithm testing and benchmarking. Conducted testing on various computational platforms to ensure scalability and compatibility.
 - c) **Testing and Benchmarking:** Benchmarked the Hartree-Fock implementation against existing quantum chemistry software (e.g., Gaussian, ORCA) to validate accuracy and efficiency. Tested algorithms with molecules of varying sizes and complexity to evaluate performance in different scenarios. Analyzed performance metrics such as execution time, scalability, and memory usage.
- **Results:** Achieved significant computational efficiency improvements in electronic structure calculations.

4. Identification of an Unknown Contaminant from Metal Cutting Fluid Lines.

- **Aim:** To investigate the composition and source of an unknown contaminant was adversely affecting the performance and stability of metal cutting fluids, aiming to provide solutions for maintaining fluid efficiency and longevity.
- **Method:**
 - a) **Sample Collection and Preparation:** Collected contaminated fluid samples from operational metal cutting lines in collaboration with **Master Fluid Solutions** (Perrysburg, OH). Conducted initial inspections, including visual observation and simple physical tests (e.g., pH, viscosity) to characterize the contaminant's basic properties.

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- b) **2D NMR Analysis:** Performed two-dimensional nuclear magnetic resonance (NMR) spectroscopy, including **COSY (Correlation Spectroscopy)**, **HSQC (Heteronuclear Single Quantum Coherence)**, and **HMBC (Heteronuclear Multiple Bond Correlation)**. Utilized these techniques to deduce structural information about the contaminant, focusing on proton-carbon connectivity and functional group identification.
 - c) **Comparative Database Analysis:** Cross-referenced the NMR data against known chemical spectra databases to narrow down potential contaminant candidates.

➤ **Results:** Successfully identified the contaminant, providing actionable insights for fluid formulation adjustments.

5. Adiabatic Photoreaction Mechanisms.

- **Aim:** To explore advancements in the understanding of adiabatic photochemical reaction mechanisms.
- **Method:** Conducted an extensive review of recent theoretical and experimental studies.
- **Results:** Summarized findings and presented them in a detailed class presentation.

ENTREPRENEURIAL EXPERIENCE

- 1. **Research and Development Engineer**, Tongling Haochen Technology Co., LTD, Tongling, China
 - a) Completed computational simulation projects for various clients;
 - b) Tutored international students in organic chemistry, focusing on theoretical concepts and problem-solving techniques.
- 2. **Lab Intern**, Shanghai Chlor-Alkali Chemical Co., LTD, Shanghai, China
 - a) Conducted molecular weight measurements of polyethylene products;
 - b) Operated analytical testing instruments for quality control, ensuring compliance with industry standards.

HONORS & SCHOLARSHIPS

- 1. Third Prize in "Challenge Cup" Chemistry Competition (Top 10%) Donghua University, 2014
- 2. The Outstanding Student Prize (First-Grade) (Top 10%) East China Normal University, 2020

TECHNICAL SKILLS

- ✧ **Quantum Chemistry Software:** Skilled in using Gaussian, ORCA, Molcas, and GAMESS for molecular modeling, quantum chemistry calculations, and dynamic simulations.
- ✧ **Programming and Technical Tools:** Proficient in Python, C++, Fortran, MATLAB, and Bash scripting, with experience in developing computational models and automating workflows.
- ✧ **Languages:** Mandarin (Native), English (IELTS 6.5).

REFERRERS

- ✧ Available upon request.