Huiwen Tan

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Education

The University of Queensland, Australia Feb. 2020 – Dec. 2024

- Bachelor of Advanced Science (Honours) in Chemistry
- **Honours Thesis:** "On-the-fly machine learning force field accelerated *ab initio* molecular dynamics for $[Fe(ptz)_6](BF_4)_2$", 50 pages
- **Coursework:** Physical Chemistry; Advanced Inorganic Chemistry; Determination of Molecular Structure; Calculus & Linear Algebra I & II; Multivariate Calculus & Ordinary Differential Equations; Quantum Mechanics I

Research Experiences

Development of On-the-Fly Machine Learning Force Fields for Spin Crossover Materials Jan. 2024 – Present

Supervised by Prof. Ben Powell and Dr Carla Verdi

- Constructed the machine learning force fields based on radial and angle descriptors by sampling of local reference configurations generated during *ab initio* molecular dynamics simulations
- Achieved the performance of force fields with the same level of accuracy as DFT in predicting spin crossover-related properties, including structural parameters of equilibrium structures in low-, intermediate-, and high-spin states, enthalpy differences, and phonon density of states for the focus materials
- Performed reference *ab initio* calculations and force field training with VASP.6

Density Functional Theory (DFT) Study of the Light-Induced Excited Spin-State Trapping Effect in Spin Crossover Materials Nov. 2022 – Jun. 2023

Supervised by Prof. Ben Powell and Dr Muhammad Nadeem

- Investigated spin crossover dynamics for phosphorene complexes $[Fe(dppen)_2X_2]$ (X = Br or Cl) in various environments from DFT calculations
- Devised a parameter-free computational scheme to model the all-atom free energy surface and kinetic barriers associated with spin-state interconversions
- Reproduced the experimentally observed trends in the influence of relaxation kinetics of the trapped excited state
- Coded and implemented resulting models using ADF2020 program on Australia National Computational Infrastructure Gadi

Stereoselective Reduction of 5-*C*-bromo-D-glucuronyl β-fluoride with the Mediation of Tributyltin Hydride: A DFT Investigation Jul. 2022 – Nov. 2022

Supervised by Prof. Elizabeth Krenske

- Identified 5 possible transition state conformers through conformational search, and determined the stereoselectivity by calculating the respective energy barriers
- Benchmarked the isomeric ratio of products, L-ido:D-gluco, using 7 exchange-correlation functionals, yielding computational results between 1:0.03 and 1:0.06 close to the experimental value of 1:0
- Conducted DFT calculations using Gaussian 16, and derived the reaction mechanism driven by the transition state gauche effect revealed from the computational results

Skills

Computational Chemistry Software: VASP, Gaussian, ADF, Quantum ESPRESSO

Programming Languages: Shell (bash), Python (NumPy, SciPy, Matplotlib, ASE, Phonopy, pymatgen), C/C++, MATLAB, R, Mathematica, LaTeX

Awards and Honours

Summer Scholarship for 2022/23 Summer Research Program — Nov. 2022

Dean's Commendation for Academic Excellence in Semester 1, 2020 — Aug. 2020

Manuscript

Tan, H.; Nadeem, M.; Powell, B. J., *Ab initio* dynamics of spin crossover complexes, equilibrium and no-equilibrium spin-transitions in $Fe(dppen)_2X_2$ (in preparation)

- **Contributions:** conceptualization, data curation, formal analysis, investigation, methodology, software, visualization, writing - original draft

Work Experiences

Casual Academics, The University of Queensland – Brisbane, Australia — Feb. 2024 – Nov. 2024

- Taught and demonstrated the laboratory sessions of a chemistry course, CHEM1100: Chemistry 1, in Semesters 1 & 2, 2024, supervised 15-20 students
- Participated in the assignments, mid- and end-of-semester exams marking and assisted in the school-based in-semester and end-of-semester exams invigilation

Administrative Intern, Beijing Genomics Institute – Shenzhen, China — Oct. 2021 – Dec. 2021

- Responsible for the laboratory management of the whole Institute of Biochemical Technology, supported the daily operation of the laboratory and administered the procurement of materials

Testing Technician, IMPAQ Testing Technology Co., LTD – Shenzhen, China — Aug. 2021 – Oct. 2021

- Third-party testing of textile products, including pH value, and the contents of formaldehyde and heavy metal