Cancan **Huang**

Graduate Student

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"Failure is the mother of success."

Summary

A current second-year graduate student in the Department of Chemistry in Brown University. I am interested in developing Quantum Monte Carlo(QMC) method for challenging tasks in quantum chemistry such as electronic structure computational methods for strongly correlated materials. Part of my project is related to the application of machine learning in QMC for a more effective and more accurate approach.

Education

Brown University

Providence, RI, U.S.A

Graduate Student — *Sept. 2017 - PRESENT*

- Advisor: Prof. Brenda Brubenstein
- Developing accurate simulation techniques for strong correlated two-dimensional materials using Quantum Monte Carlo
- Developing machine-learning techniques optimized for the exscale computing of chemical systems

Fudan University

Shanghai, China

Undergraduate Student — *Sept. 2013 - July 2017*

- Advisor: Prof. Junli Hou
- Bachelor of Science in Chemistry, Department of Chemistry. GPA: 3.49/4.00
- Outstanding student of Department of Chemistry (based on Research Ability and GPA)

The University of Auckland

Auckland, New Zealand

Exchange Student — *Feb. 2016 - July 2016*

- Exchange student, Department of Chemistry
- Referred by Fudan University based on academic record and extra-curricular experience

The University of Hong Kong

Hong Kong, China

Summer Student — *July 2015 - Aug. 2015*

- HKU summer program in Chemical Biology
- Referred by Department of Chemistry of Fudan University

Honors & Awards

2017	**Outstanding Undergraduate Award**, Department of Chemistry	*Fudan University*
2016-2017	**The Second-Class Scholarship for Outstanding Students**, Department of Chemistry	*Fudan University*
2015-2016	**Thermo Fisher STEM Scholarship**, Department of Chemistry	*Fudan University*
2016	**Excellent Poster Award in the 4th Undergraduate Technology & Academy Forum**, Department of Chemistry	*Fudan University*
2014-2015	**Thermo Fisher STEM Scholarship**, Department of Chemistry	*Fudan University*
2014-2015	**The Second-Class Scholarship for Outstanding Students**, Department of Chemistry	*Fudan University*
2014-2015	**GRA Special Talent Scholarship**, Department of Chemistry	*Fudan University*
2014-2015	**Professional Fellowship**, Department of Chemistry	*Fudan University*
2013-2014	**Thermo Fisher STEM Scholarship**, Department of Chemistry	*Fudan University*
2013-2014	**The Third-Class Scholarship for Outstanding Students**, Department of Chemistry	*Fudan University*

Research Experience

Bridging the Time Scale in Exa-scale Computing of Chemical Systems

Providence, RI, U.S.A

Graduate student, Department of Chemistry, Brown University — *Dec. 2018 - present*

- Apply machine learning using auxiliary-field quantum Monte Carlo simulations to sample the many-body system
- Accelerate the construction of quantum Monte Carlo propagators with machine learning techniques

Ab initio Study of CH_3I Rydberg States with Spin-Orbit Coupling

Providence, RI, U.S.A

Graduate student, Department of Chemistry, Brown University — *May 2018 - Dec. 2018*

- Multireference configuration interaction (MRCI) *ab initio* calculations with/without spin-orbit coupling were performed using the MOLPRO package on the valence and 6s and 6p Rydberg bands of the CH_3I molecule
- Previous experimental peaks were fit to a C-I distance using the calculated repulsive valence state surfaces and ion ground state surface, whose curvatures resemble those of the Rydberg states from the calculation

Synthesis of Pillar[5]arene with Diynes Side Chain Structure

Shanghai, China

Research Assistant Department of Chemistry, Fudan University — *Jan. 2017 - June 2017*

- Advisor: Prof. Junli Hou
- Synthesis of a pillar[5]arene with novel side chain structure containing diynes was conducted
- Possible synthetic paths are proposed and lessons are gained for later studies

Biosynthesis of Morphine

Montreal, Canada

Research assistant Department of Chemistry, McGill University — *July 2016 - Sept. 2016*

- Supervisor: Professor Jean-Philip Lumb
- Assisted with the synthesis of morphine materials and product separation as well as characterization
- Applied different separation technology according to properties of different products such as column chromatography and recrystallization

PH Control Artificial Transmembrane Proton Channel

Shanghai, China

Research Assistant Department of Chemistry, Fudan University — *Apr. 2015 - Jan. 2016*

- Advisor: Prof. Junli Hou
- Independently conducted the synthesis and characterization of bi-functionalized pillar[5]arene as well as optimized and simplified the synthesis route
- Workded on introduction of imidazole group into pillar[5]arene backbone aiming to control the switch of the channel under the difference of voltages
- Improved the side chain structure based on the result of X-ray diffraction and the path clamp technique.

Presentation

Ab initio Study of CH_3I Rydberg States with Spin-Orbit Coupling

Orlando, FL, U.S.A

Poster Presentation for 2019 ACS National meeting & Expo — *March, 2019*

- Multireference configuration interaction (MRCI) *ab initio* calculations withwithout spin-orbit coupling were performed using the MOLPRO package on the valence and 6s and 6p Rydberg bands of the CH_3I molecule as a function of the methyl-iodine distance with frozen C_3v geometry.
- Previous experimental peaks were fit to a C-I distance using the calculated repulsive valence state surfaces and ion ground state surface. Transition dipole moments between repulsive valence states and Rydberg states show that the $6s_{1/2}$ and $6p_{1/2}$ Rydberg states possess significant transition moments with the ${}^3Q_0^+$ repulsive state.

Spin-Orbit Coupling – An Important Relativistic Effect

Providence, RI, U.S.A

Oral Presentation for Brown University Chemistry Department's Physical Chemistry Tea Session — *Oct. 18th, 2018*

- Introduced the origin and quantum computer applications of spin-orbit coupling. Computational methods for spin-orbit coupling have been discussed and its calculation of methyl iodide is presented.

Synthesis of Bi-functionalized Pillar[5]arene

Shanghai, China

Poster Presentation for Fudan University Chemistry Department's 4th Undergraduate Technilogy&Academy Forum — *April, 2016*

- Introduced the synthesis of bi-functionalized pillar[5]arene and its potential application in chemical biology.

Extracurricular Activity

Language Ability

English

- GRE: Verbal 152/170 + Quantitative 168/170(95%) + Writing 3.5/6.0
- TOEFL: 102/120 (Writing: 29/30) Reading: 29/30

Computer Skills

(if applicable: N -Novice, P - Proficient, A - Advanced)

- Chemical software: ChemBioDraw, Maple, Matlab, Mathematics
- Office: Microsoft Office, Adobe Photoshop, Sublime Text 3, Endnote, Zotero, Refworks
- Programming Languages: Python, Linux, C, Matlab, R