# Yuquan Cao

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## EDUCATION

**Zhiyuan College, Shanghai Jiao Tong University (SJTU), China** 09/2014 - 06/2018

- Major: Chemistry, Candidate for Bachelor of Science
- Overall GPA: 85/100; 3.3/4.0

**STEP (Short Term English Program) at University of Washington, Seattle, United States** 08/2016

**Pre- Master Program at International College of the University of Southern California** 09/2018 - 12/2018

**Master Program at Viterbi College of the University of Southern California** 01/2019- 05/2020

- Major: Material Engineering
- Overall GPA: 3.6/4.0

**Chemistry PhD program at the New York University Shanghai** 06/2020 - present

- Major: Computational Chemistry
- Present GPA: 4.0/4.0

## RESEARCH EXPERIENCE

**Researcher, Force Field Development for Macromolecular Coarse Graining, SJTU** 10/2017-05/2018

Undergraduate Thesis Supervisor: Huai Sun

- Developed coarse grained model for macromolecule polystyrene and calculated its thermodynamic properties, such as density, turning radius, RDF, glass transition temperature, surface tension and etc.
- Verified all the thermodynamic properties of all-atomic force field, obtained coarse graining force field parameters according to the Boltzmann Inversion, debugged the parameters according to the molecular dynamics simulation of coarse graining force field, as well as came up with the coarse graining model with temperature mobility and complying with its structures
- Read literature, grasped relevant software and data processing methods, compiled the experimental data and wrote the graduation thesis

**Teaching Assistant, Zhiyuan College, SJTU** 09/2017-01/2018

- Assisted the professor in the selection and grading of assignments and examination papers, answering students' questions, attendance recording and making teaching PPT
- Guided students who interested in computational chemistry to visit the lab and solved their problems

**Researcher, Theoretical Chemistry Lab, SJTU** 10/2015-05/2018

- Worked with Doctor Shen, Zhe to carry out the research on the self-assembly simulation and CMC prediction of surfactant and the coarse-grained field of benzene
- Independently conducted the force field development of ethylene glycol and applied GAUSS to find out ten possible optimum configuration
- Gained preliminary understanding and application of enhanced sampling method, Monte Carlo Method and coarse-grained force field

**Researcher, Theoretical Chemistry Lab, SJTU** 07/2019-08/2019

- Worked with Doctor Evangelia Charvati to carry out the research on the automatically mapping method for coarse graining models. We use the centrality method to calculate and compare the importance of each atom of the molecule to automatically get coarse-grained beads of the macromolecule.

**Researcher, USC**

- During the spring and fall semester in USC, I took MASC 575 and MASC 576. In MASC575, I did two projects: calculating the properties of this FCC crystal; using Monte Carlo method to calculate the value of π through two ways and the application of the Metropolis Algorithm. In MASC576, I have done two projects: calculate the properties of Cu; nanoindentation of Cu.

**Researcher, NYU Shanghai**

- I am now doing research in Prof. William J. Glover's group. The research topic is to explore the charge transfer and energy transfer mechanism in photosynthesis system. We want to build an exciton model which can systematically be improvable by considering interaction between pairs of multiple monomers.

## ACTIVITIES

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| Organizer, The International Conference on Molecular Simulation, ICMS-2016 | 10/2017 |
| Member, Youth Volunteer Service Group, SJTU | 09/2014-09/2015 |
| Editor, Yiyou Newspaper, SJTU | 09/2014-02/2016 |
| Minister, Public Relations Department of Students Union, SJTU | 09/2014-02/2015 |

## HONORS AND AWARDS

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| School Excellent Member, Youth League Committee, SJTU | 03/2017 |
| Zhiyuan Honorary Scholarship, Zhiyuan College, SJTU | 08/2016 |
| School-level Third-class Scholarship, SJTU | 08/2016 |
| Zhiyuan Honorary Scholarship, Zhiyuan College, SJTU | 02/2016 |
| School-level Third-class Scholarship, SJTU | 02/2016 |

## SKILLS

Proficient in programming language Python and Software LAMMPS, GROMACS, Amber, Q-chem, Psi4, Gaussian, Materials Studio and Matlab.