Kecai Xuan

Curriculum Vitae

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EDUCATION

JUL.2023 – PRESENT **Research Intern**
Department of Chemistry
University of Wisconsin - Madison

SEP.2020 – PRESENT **Undergraduate**
Department of Chemical Physics
University of Science and Technology of China

Major: Chemical Physics, **Overall GPA**: 3.68/4.30, **Ranking**: 16/105

LITERATURE

Book: Introduction to Statistical Mechanics

Notes for Statistical Mechanics, highlighting on conceptual consistency, logical coherence, and full of insights and discussions. Still under construction; available online at **Github**.

Article: The Analysis of USTC

Critical thoughts towards the rat race at our school, analyzed the cause and effect, claiming that the Truth and Liberty shall become our unshakable belief. Available online at **USTC Forum**.

Article: The Faults of Zhiyong

Discussed the Org.Chem lecturer's misconducts in classical Chinese, reported this to the Forum of Students and Teachers and received commendation. Available online at **icourse.club**.

ACTIVITIES

OCT.2023 **Organizer of Monthly Reading, Student Union**

1. Discussed with the lecturer and polished the event copy.
2. Prepared the event and the venue.

OCT.2022 **Volunteer of the Chunlei Program, Student Union**

1. Helped collect and sell secondhand books at school.
2. Organized the charity sale for children in remote area.

MAR.2022 - SEP.2022 **Member of School Dancing Association**

1. Participated in the dancing teaching course as a learner.
2. Joined the ballroom dancing parties organized by the university.

SEP.2021 - SEP.2022 **Co-Captain of Frisbee School Team**

1. Second Prize, Shanghai Ultimate Frisbee Hat Competition, 2022.
2. Joined the exchange competition between USTC and HFUT.

SKILLS

EXPERT Mathematica, C#, LaTeX, Python

INTERMEDIATE Linux, MATLAB, LAMMPS, Gaussian

RESEARCH

Ab Initio Raman Spectra Calculation

1. Reviewed the theory of light scattering and the basic relationship between the Raman polarizability tensor and the molecular states.
2. Identified the difference prefactor between classical correlation and quantum correlation for the AIMD method.
3. Implemented polarizability calculations with PySCF.
4. Modified the PySCF package for Raman activity calculation.

Supported by: CIEE, USA.
Supervisor: **Prof. Yang Yang**, TCI, UW-Madison
Mid Report: **Basic Theory of Raman Spectroscopy**
Final Report: **Codes for Static Raman Calculation**

Physicochemical Properties of Bio-Phase Transitions

1. Simulated the liquid-liquid phase separation (LLPS) phenomenon in bio-systems.
2. Drew and discussed the phase diagram of the LLPS.
3. Estimated and calculated the transport properties of the separated droplets.
4. Investigated and the mechanism of LLPS and speculated its relationship to the intercellular reaction and function.

Supported by: Ministry of Education, China.
Supervisor: **Prof. Zhonghuai Hou**, SCMS, USTC.
Final Report: **Liquid-Liquid Phase Separation**

SELECTED AWARDS

2023 **Chen Linyi Scholarship**
Mr. Chen Linyi

2022 **Outstanding student scholarship**
University of Science and Technology of China

2022 **Excellent Student Scholarship of GIES**
Guangzhou Institute of Energy Conversion, CAS

2021 **Huang Minglong Scholarship of SIOC**
Shanghai Institute of Organic Chemistry, CAS

2021 **Scholarship of Lu Jiaxi Talent Program**
University of Science and Technology of China

2021 **2nd Prize, Chinese Mathematics Competition**
Chinese Mathematical Society