

# 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 and logical coherence, full of insights and discussions. Still under construction, available online at [Github](#).

### Article: The Analysis of USTC

Critical thoughts towards the rat race in 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

Pointing out the Org.Chem lecturer's misconducts in classical Chinese, reported this to the Forum of Students and Teachers and received cheers. 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 collecting and selling the second-hand books at school.
  2. Organized the charity sale for the 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. Found the difference prefactor between classical correlation and quantum correlation for AIMD method.
3. Implemented polarizability calculation of CNEO with PYSCF package.
4. Modified Atomic Simulation Environment for Raman Spectra calculation.

**Supported by:** CIEE, USA.

**Supervisor:** Prof. **Yang Yang**, TCI, UW-Madison

**Mid Report:** **Basic Theory of Raman Spectroscopy**

**Final Report:** **AIMD Raman Spectra Calculation**

### Physicochemical Properties of Bio-Phase Transitions

1. Simulated the liquid-liquid phase separation (LLPS) phenomenon in bio-systems.
2. Drawn and discussed the phase diagram of the LLPS.
3. Estimated and calculated the transport properties of the separated droplets.
4. Investigated the mechanism of LLPS, speculated the 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** (10%)  
*Mr. Chen Linyi*
- 2022 **Outstanding student scholarship** (10%)  
*University of Science and Technology of China*
- 2022 **Excellent Student Scholarship of GIES** (10%)  
*Guangzhou Institute of Energy Conversion, CAS*
- 2021 **Huang Minglong Scholarship of SIOC** (10%)  
*Shanghai Institute of Organic Chemistry, CAS*
- 2021 **Scholarship of Lu Jiaxi Talant Program** (5%)  
*University of Science and Technology of China*
- 2021 **2nd Prize, Chinese Mathematics Competition**  
*Chinese Mathematical Society*