

## Yu Wang

Email: zju\_wangyu@zju.edu.cn

Address: HangZhou China

Age: 26      Gender: Male

Current Status: Research Assistant



## EDUCATION & WORK

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<b>Zhejiang University</b> - Department of Chemistry	2023 - 2024
Research Assistant	HangZhou China
<b>Zhejiang University</b> - Department of Chemistry	2020 - 2023
Master (Chemistry)	HangZhou China
<b>China Pharmaceutical University</b> - Faculty of Engineering	2016 - 2020
Bachelor (Pharmacy)	NanJing China

## HONORS & AWARDS

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Jiang Zhi Modern Biological and Pharmaceutical Technology Research Award	2023
The Second Prize Scholarship Award	2022
The Assistantship Award	2022
Rank NO.1 in the Zhejiang University Graduate Entrance Examination	2020
The Third Prize Scholarship Award	2019
The Third Prize Scholarship Award	2017

## RESEARCH EXPERIENCE

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### **Molecular Dynamics Simulation of Adsorption Mechanism of**

### **Coagulation Factor Xa on Na<sup>+</sup> Exchange Zeolite Surface**

*Project Continuer*

Investigating the adsorption behavior of coagulation factor FXa light chain and the coagulation factor FXa-FVa complex on NaY or CaY zeolite surfaces with varying degrees of ion exchange. This study aimed to elucidate the roles of different metal ions in the binding process of coagulation factor FXa to Hemostatic zeolite surfaces.

### **Exploration of the catalytic mechanism for the**

### **Dissociation of H<sub>2</sub>O<sub>2</sub> by bimetallic Au/Pd nanoparticles**

*Responsible for computational aspects*

using DFT to explore the absorption energies of H<sub>2</sub>O<sub>2</sub> on surfaces with different ratios of Au/Pd, to predict the Au/Pd nanoparticles with optimal performance. Constructing advantageous adsorption configurations of H<sub>2</sub>O<sub>2</sub> on different surfaces. Subsequently, possible routes and corresponding free-energy profiles of dissociating H<sub>2</sub>O<sub>2</sub> will be compared between the pure Au surface and the Au/Pd mixed surface, which aims to infer the promoting effect of heteronuclear metal sites on the reaction.

### **Molecular Dynamics Simulation for Constructing a Drug Delivery System**

### **using Folic Acid-Modified Natural Silk Fibroin Protein**

*Responsible for computational aspects*

Conducted protein structure simplification, peptide chain construction, folic acid-modified peptide chain construction, and simulation of their conformational changes in both aqueous and methanol solvents.

Investigated interactions between peptide chains and drugs, as well as interactions between peptide chains and cell membranes.

### **An Engineered Design of Self-assembly Nanomedicine Guided by Molecular**

**Dynamic Simulation for Photodynamic and Hypoxia-directed Therapy** [10.1021/acs.molpharmaceut.2c01079](https://doi.org/10.1021/acs.molpharmaceut.2c01079)

*First Author*

2021 - 2023

Synthesized hypoxia-responsive prodrug by attaching hypoxic moiety to docetaxel. Selected amphiphilic photosensitizers for drug delivery system construction. Validated and explained binding using molecular dynamics simulations. Visualized self-assembly and structure through coarse-grained simulation.

### **Investigation of Fe/Ni Nanocatalytic Systems in Aqueous Micelles**

*Main Team Member*

2018 - 2019

Responsible for the preparation of Fe/Ni nanomicelles and testing their catalytic performance, such as Suzuki coupling reactions.

## **THESES**

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**Master:** Study on Light-Enhanced Nanomedicine Delivery System in Response to Tumor Micro-Environment

**Bachelor:** Palladium-Catalyzed Defluorination Dearomatization of gem-Difluorinated Cyclopropanes with  $\beta$ -Naphthols

## **SKILLS**

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**Language:** IELTS 6.5

(Listening: 6.0, Reading: 7.0, Speaking: 6.0, Writing: 6.0)

**Software:** Gromacs, Gaussian, LAMMPS, VASP, Quantum ESPRESSO, CYLview, Pymol, VMD, AutoDock, Materials Studio, Amber, Java, Python, Prism, Origin, Photoshop, etc.