My name is Yixuan Pu. I obtained my bachelor’s degree in Chemistry from Lanzhou University, China and will gain my master’s degree in Physical Chemistry at the University of Science and Technology of China. My work is focusing on solving catalytic issues with computational methods. I am interested in using first-principles computational modeling and machine learning approaches to understand and predict catalysts for use in energy storage, sustainable chemical production and reducing the environmental impact of products. Leveraging the machine learning algorithms, I will be able to analyze experimental data and identify the key factors that influence the catalytic performance, such as size effect and the interaction between catalyst and support.

**RESEARCH EXPERIENCE**

**Exploring the Actual Structure of Alloy Clusters During ORR Reactions**

*Independent Research. Supervisor: Prof. Weixue Li and Prof. Jinxun Liu Mar. 2022 – present*

* Applied theoretical method to validate the migration process observed during AIMD simulations and to quantify the reactivity of the dpoed metal atoms from subsurface to alloy cluster surface.
* Used Density Functional Theory (DFT) calculations to determine the oxygen absorption energy on two clusters
* Studied 55-atom AgCo bimetallic cluster for its enhanced fluidity, which facilitates the understanding of the cluster reconstruction dynamics and identified the actual active site by computing the ΔG of Oxygen reduction reaction (ORR) intermediates
* Expanded the scope of study to encompass 30 randomly selected alloy cluster combinations, 20 of which involved the migration of doped metal atoms to cluster’s surface from inside
* Generated datasets through first principle calculations, applied machine learning technique to establish the connection between ORR activity of SAAs and potentially related features, illuminating the key determinants of ORR activity of SAAs
* Predicted noble mental free high-performance SAAs catalyst with this method

**Investigation of Ordered PtNiM Alloy Nanoparticles as High-Performance ORR Catalysts**

*Core Research Member. Supervisor: Prof. Haiwei Liang Nov. 2021 – Nov. 2022*

* Leveraged computational techniques to investigate how the addition of different dopant metals varies the degree of order in PtNi alloys
* Utilized VASP to generate training set and then fit Cluster Expansion (CE) model
* Conducted structural searches using genetic algorithm (GA), which yielded the stable structure of PtNiM with the lowest energy
* Explored the factors that influenced the formation energy of alloy by studying alloy structures and Bader charge analysis
* Discovered a strong linear relationship between the electrostatic interactions of Pt with the dopant elements in the alloy and the formation energy of the ternary alloy

**Studying the Mechanism of High-Entropy Alloy Catalyzed Hydrogen Evolution Reaction**

*Undergraduate Thesis, Supervisor: Prof. Jinxun Liu Mar. - May 2020*

* Utilized VASP to calculate the adsorption energy and free energy of hydrogen (H) atoms on various metal surfaces, as well as computed electric current density; investigated the relationship between ΔGH (Gibbs free energy change) and electric current density
* Explored the influence of water absorption ability of different alloys on the hydrogen evolution reaction by calculating water adsorption energy on ten distinct metal surfaces.
* Examined the impact of high-entropy alloy on water molecule dissociation by employing the Climbing Image-Nudged Elastic Band (CINEB) method to study the transition states of the reaction
* Conducted frequency analysis to validate the credibility of these transition states and analyzed the activation energy and reaction enthalpy for the dissociation of water on various metal surfaces.

**Research on the Preparation of Vertical Graphene (VG) and Its Application**

*Independent Researcher Nov. 2020 - Aug. 2021*

* Conducted a review of previous research on allotrope of carbon elements, especially fullerene, carbon nanotube and graphene
* Explored the growth mechanism of VG and the [Plasma Enhanced Chemical Vapor Deposition](https://www.sciencedirect.com/topics/engineering/plasma-enhanced-chemical-vapor-deposition" \l ":~:text=PECVD%20is%20a%20CVD%20process,From%3A%20Energy%20Materials%2C%202021) (PECVD) method, most widely used to produce VG of high quality, examined the factors that influence VG growth including plasma source, temperature, pressure, carbon source, gas proportion, VG morphology and many other properties
* Summarized the VG's distinctive characteristics, such as exposed and ultra-thin graphene edges, vertical orientation, non-stackable morphology, and high carrier mobility, and its wide applications in sensing and electro-chemical devices

**Investigation on the Water Quality and Air Quality of the Yellow River in Lanzhou City**

*Social Practice Project. Supervisor: Prof. Haixia Zhang Jul. 2019*

* Investigated the hardness of Yellow River's water and its chemical oxygen demand (COD), a key indicator of water quality
* Measured the hardness COD levels by using EDTA complexometric titration method and potassium permanganate titration method respectively
* Conducted a secondary assessment of water hardness using Coupled Plasma-Atomic Emission Spectroscopy (ICP-AES)
* Experiments proved that the hardness of the river was far lower than the recommended drinking water standards but the water's oxygen demand was at a favorable level

**Study on the Ratio Fluorescent Sensor of Metal Organic Framework (MOFs) with Guest Encapsulation**

*Independent Research. Supervisor: Prof. Weisheng Liu Mar. - Dec. 2019*

* Studied literature to familiarize the MOFs, their unique properties and applications
* Designed a comprehensive study to investigate MOFs' potential for detecting trinitrotoluene (TNT), completed MOFs manufacture, guest fluorescence encapsulation, and luminescent property test
* Synthesized fluorescent sensor with high selectivity (1μmol/L) by encapsulating Ru(bpy)3 within IRMOF-9 and gained a good linearity

**AWARDS & HONORS**

* Third Prize at National Chemistry Competition for College Students 2018
* Second Prize at “Chemistry Around Us” Knowledge Competition, Lanzhou University 2017
* Second Prize at English Presentation Contest, Lanzhou University 2017
* First Prize at National Chemistry Competition for High School Students, Jiangsu Province 2016

**LEADERSHIP EXPERIENCE AND VOLUNTEERING**

* Poverty Situation Investigation in Rural Areas in Hubei and Anhui in China, 2020
* Joined a research program held by Zhejiang Xingchuang Public Welfare Foundation to investigate rural household poverty in these two provinces by designing a survey, collecting and analyzing data, and exploring possible solutions for poverty alleviation
* English-version College Website Development, 2019
* Assisted in building an English version website of Cuiying Honors College by translating all Chinese content, Lanzhou University and composed articles covering news, events and student achievements
* Student Leadership Experience in University-level and Department-level Student Union, 2018-2020
* Collaborated with other students to plan and organize students’ events and improve integration and sense of belonging
* Volunteering at Yan Qiao Nursing Home, 2016
* Volunteered once a month, providing assistance, companionship, and support to the elderly residents

**SKILLS & HOBBIES**

* **Computer Software:** Proficient in simulation software (VASP, Material Studio, Gaussian, etc.) and machine learning packages (Sklearn, PyTorch, etc.)
* **Hobbies:** Bamboo Flute (Gain the highest level - Performance Level 10), Football, Basketball, e-sports, Stage Drama (Leading actor in several classic plays since high school), Traveling