

# Zhe (Cyril) Xu

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## Education

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### University College London, UK

*(December 2021 – Present)*

- PhD in Chemistry

### University College London, UK

*(October 2020 – October 2021)*

- MSc. Molecular Modelling (Distinction)

### Imperial College London, UK

*(October 2016 – July 2020)*

- BSc. Chemistry with Management (High Upper-Second Class)

### London School of Economics and Political Science, UK

*(July 2018 - August 2018)*

- Summer Programme: Strategic Management

### Abbey College Cambridge, UK

*(September 2014 – June 2016)*

- A-levels: Mathematics: A\*, Chemistry: A, Physics: A

## Research Experience

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### Postgraduate Researcher, Dr Robert G. Bell, University College London, UK

*(October 2020 – October 2021)*

- Computationally studied the CO<sub>2</sub>/H<sub>2</sub>O competitive adsorption in defective Metal-organic Frameworks (MOFs) using periodic DFT and Monte-Carlo simulations
- Investigated how structural and electronic properties of defective MOFs affect the adsorption capacity and selectivity
- Aimed to propose strategies for the reticular design and synthesis of novel functional materials for carbon capture and conversion

### Undergraduate Researcher, Prof. Patricia A. Hunt, Imperial College London, UK

*(February 2019 – March 2019)*

- Modelled and predicted the formation of Boron-Phosphorous Frustrated Lewis Pairs (FLP) by DFT
- Investigated the importance of non-covalent intermolecular interactions between Hydrogen atoms in FLPs
- Tabulated, analysed and visualised experimental data by Python

### Inorganic Laboratory Assistant, Prof. Hongwei Hou, Zhengzhou University, China

*(July 2016 – August 2016)*

- Reviewed existing literatures on synthetic targets
- Prepared NMR data for individual products

## Other Experience

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### **Specialist, Apple, Regent Street, London, UK**

*(October 2021 – Present)*

- Uncover customers' needs and provide exceptional services by creating excitement around Apple products, presenting the right solutions that enrich customers' life
- Actively educate customers about product features and the Apple ecosystem across the product line
- Assist team members in visual merchandising and backstage stock replenishments
- Very high Net Promotor Score (100/100) and positive customer feedbacks

### **Department Open Day Volunteer, Imperial College London, UK**

*(June 2019 – September 2019)*

- Demonstrated undergraduate laboratory experiments
- Presented personal experiences to 50+ audience by PowerPoint
- Assisted organisers in logistics

### **Customer Host, Fortnum & Mason, London, UK**

*(November 2018 – April 2019)*

- Customer engagement in professional manners at a high-end retail establishment
- Coordinated with other departments to ensure adequate stock level

### **General Assistant, Loon Fung Chinatown, London, UK**

*(February 2018 – August 2018)*

- Negotiated prices with buyers and suppliers and built sustainable client relationships

### **Front Desk Volunteer, Commemoration Day 2017, Imperial College London, UK**

*(October 2017)*

- Assisted disabled guests to correct venues

## Events

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### **Participant, Protein Structure Fundamentals: Searching – Analyzing – Modelling de.NBI workshop, Hamburg, Germany**

*(September 2019)*

### **Participant, RDKit User Group Meeting 2019, Hamburg, Germany**

*(September 2019)*

### **Participant, Milestones in Molecular Simulations Symposium, Imperial College London, UK**

*(June 2019)*

## Skills and Interests

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### **Computer:**

- DFT: Gaussian, CP2K, NWChem
- Empirical: GULP, DL-POLY
- Monte-Carlo: DL-MONTE
- General programming: Python (Intermediate), Fortran 90 (Elementary)
- High Performance Computing
- LaTeX

**Languages:**

- Chinese (Native)
- English (Fluent)
- German (Elementary)

**Interests:**

- Swimming
- Hiking
- Travelling

**References**

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Available upon request