

# Jiawei Zhan

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## EDUCATION

### University of Science and Technology of China (USTC)

- **Major:** Physics

Sep. 2016 - present

Major GPA: **3.72/4.3**

### University of California, Los Angeles (UCLA)

- School of Physics

Jun. 2018 - Aug. 2018 summer session

Overall GPA: **4.0/4.0**

#### Course Highlights:

Atomic Physics (97, first in the class)	Electrodynamics (92)
Thermodynamics and Statistical Physics A (90)	Solid physics A (93, top5 in the class)
Equations of Mathematical Physics A (91)	Probability Theory and Mathematical Statistics (92)
Theoretical Mechanics A (95, top3 in the class)	Computer Programming A (90)

## PUBLICATION

- Shuhui Wang, **Jiawei Zhan**, Kui Chen, Asad Ali, Linghui Zeng, He Zhao, Wanglai Hu, Lixin Zhu, Xiaoliang Xu. *Potassium-doped g-C<sub>3</sub>N<sub>4</sub> Achieving Efficient Visible-Light-Driven CO<sub>2</sub> Reduction* (Submitted to Journal: CARBON)
- A Python Package for Lattice and Surface Matching of Epitaxial Interfaces: Organic Interfaces (*be in preparation*)

## RESEARCHES

### ❖ Research Assistant, Carnegie Mellon University (CMU)

Department of Material and Science Engineering

Project: **A Python Package for Lattice and Surface Matching of Epitaxial Interfaces: Organic Interfaces**

Advisor: Dr. Noa Marom

Jul. 2019 – Sep. 2019

*Summary: Designed and implemented a state-of-the-art python package for predicting the most likely structure of organic interfaces.*

- Designed a graph-theory algorithm for efficient slab generation, which outperformed all previous algorithms in conserving the molecular number and structures as well as mechanical properties
- Implemented a lattice matching algorithm for optimizing the lattice parameters of new interfaces and the coordinates of every atom
- Created a Graphic Neural Network (GNN) model for predicting organic systems' non-bonded interactions, with the efficiency of empirical methods and the accuracy of DFT method
- Used three different workflows to optimize the structure of interfaces, and GNN exceeded others in accuracy and time cost (Errors < 3%, 10000 × faster than DFT)

### ❖ Research Assistant, University of Science and Technology of China (USTC)

School of Physics

Project: **Potassium-doped g-C<sub>3</sub>N<sub>4</sub> Achieving Efficient Visible-Light-Driven CO<sub>2</sub> Reduction**

Advisor: Dr. Jin Zhao

Mar. 2019 – Jul. 2019

*Summary: Improved the efficiency of CO<sub>2</sub> photoreduction by doping alkali metal element to engineer the electronic properties of the catalyst*

- Found the most stable relaxed configuration of the potassium-doped g-C<sub>3</sub>N<sub>4</sub> and predicted the most practicable doping density as a reference for the experiment
- Theoretically proved that potassium doping changes monolayer g-C<sub>3</sub>N<sub>4</sub> from indirect gap to direct gap
- Calculated numerically the formation energy and Gibbs free energy ( $\Delta G_H$ ) of hydrogen atom adsorption on g-C<sub>3</sub>N<sub>4</sub> and K-doped g-C<sub>3</sub>N<sub>4</sub>, proved that the CO<sub>2</sub> reduction with K-doped g-C<sub>3</sub>N<sub>4</sub> is more efficient than that with ordinary pristine g-C<sub>3</sub>N<sub>4</sub>
- Used differential charge density to numerically prove that K-doping alters the charge distribution of g-C<sub>3</sub>N<sub>4</sub> and inhibit the electron-hole pair recombination

### ❖ Research Assistant, University of Science and Technology of China (USTC)

School of Physics

Project: **Partially Oxidized SnS<sub>2</sub> Atomic Layers Achieving Efficient Visible-Light-Driven CO<sub>2</sub> Reduction**

Advisor: Dr. Jin Zhao

Sep. 2018 – Jan. 2019

*Summary: Numerically proved that oxygen doping could enhance SnS<sub>2</sub>'s photocatalytic property in visible-light-driven CO<sub>2</sub> reduction*

- Analyzed the electronic structure and magnetic properties of O-doped SnS<sub>2</sub> and Ni-O-doped SnS<sub>2</sub> via DFT, proved that oxidation had impact on charges' distribution
- Proved numerically that oxygen-doping made Sn the binding sites of the reaction and could decrease formation energy of a significant step that influenced the whole CO<sub>2</sub> reduction process
- Calculated the optimized structure of different doped SnS<sub>2</sub> to quickly predict whether the novel materials could be produced in experiment

## AWARDS

- **2019, 2018 Bronze Award (top 20%)**, USTC Outstanding Student Scholarship
- **2018 Grand Prize (top 1%)**, The 14th USTC Physics Research Experimental Paper Competition
- **Second Prize (rank 39th)**, 30th Chinese Mathematics Olympiad, Sichuan Province

## SKILLS

- **Programming:** Python, C/C++, Java, MATLAB, Mathematica, Latex
- **Software:** VASP, FHI-aims, VESTA, Mathematica, MATLAB, Vim, Material Studio
- **Standard English Test:** TOFEL: 99 (MyBest Score: 108 -- Reading 28, Listening 26, Speaking 27, Writing 27)  
GRE: 150 (Verbal) + 170 (Quantitative) + 3.5 (AW), GRE Physics : 940

## LEADERSHIP & ACTIVITY

- Lead the class to get the **Excellent Class Award** of the Year 2017 and 2018 (top 5%)
- **2017 4th Prize**, Champion Cup (Soccer Competition for College Teams)