Jiawei Zhan

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EDUCATION

University of Science and Technology of China (USTC) *Sep. 2016 - present*

- **Major:** Physics — Major GPA: **3.72**/4.3
- **Minor:** Computer Science

University of California, Los Angeles (UCLA) *Jun. 2018 - Aug. 2018 summer session*

- School of Physics — Overall GPA: **4.0**/4.0

Course Highlights:

Atomic Physics (97, first in the class)
Thermodynamics and Statistical Physics A (90)
Equations of Mathematical Physics A (91)
Theoretical Mechanics A (95, top3 in the class)
Electrodynamics (92)
Solid physics A (93, top5 in the class)
Probability Theory and Mathematical Statistics (92)
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_3N_4 Achieving Efficient Visible-Light-Driven CO_2 Reduction* (Accepted by *Journal: ACS Sustainable & Engineering on May 20th, 2020*)
- Shuyang Yang, Imanuel Bier, Wen Wen, **Jiawei Zhan**, Saeed Moayedpour, and Noa Marom. *Ogre: A Python Package for Molecular Crystal Surface Generation with Applications to Surface Energy and Crystal Habit Prediction (Accepted by Journal of Chemical Physics on May 28th, 2020)*

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 atom numbers 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_3N_4 Achieving Efficient Visible-Light-Driven CO_2 Reduction**
Advisor: Dr. Jin Zhao *Mar. 2019 – Jul. 2019*
Summary: Improved the efficiency of CO_2 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_3N_4 and predicted the most practicable doping density as a reference for the experiment
- Theoretically proved that potassium doping changes monolayer g-C_3N_4 from indirect gap to direct gap
- Calculated numerically the formation energy and Gibbs free energy (ΔG_H) of hydrogen atom adsorption on g-C_3N_4 and K-doped g-C_3N_4, proved that the CO_2 reduction with K-doped g-C_3N_4 is more efficient than that with ordinary pristine g-C_3N_4
- Used differential charge density to numerically prove that K-doping alters the charge distribution of g-C_3N_4 and inhibit the electron-hole pair recombination

❖ Research Assistant, **University of Science and Technology of China (USTC)**
School of Physics
Project: **Partially Oxidized SnS_2 Atomic Layers Achieving Efficient Visible-Light-Driven CO_2 Reduction**
Advisor: Dr. Jin Zhao *Sep. 2018 – Jan. 2019*
Summary: Numerically proved that oxygen doping could enhance SnS_2's photocatalytic property in visible-light-driven CO_2 reduction

- Analyzed the electronic structure and magnetic properties of O-doped SnS_2 and Ni-O-doped SnS_2 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_2 reduction process
- Calculated the optimized structure of different doped SnS_2 to quickly predict whether the novel materials could be produced in experiment

PROJECT

❖ Research Intern, **Chinese Academy of Science**
Institute of Software
Project: **Dynamics Index Update of Moving Taxi**
Advisor: Dr. Limin Guo *Jul. 2017 - Aug. 2017*
Summary: Created high-efficient algorithms to implement real-time updating locations of taxis and find the nearest taxi for every user in Beijing

- Constructed the database in a tree form, largely decreasing the time spending on data's iterations
- Established the foundation of Bitmap indexing technique for taxis' locations by changing 2D coordinates to linear list
- Used Binary heap, Hash table, B tree and doubly linked list to quickly check, update (insert) or pop out targets from millions of locational data

AWARDS

- **2019 Award** (**top 20%**), USTC Outstanding Student Scholarship
- **2018 Award** (**top 20%**), USTC Outstanding Student Scholarship
- **2018 Grand Prize** **(top 3%),** The 14th USTC Physics Research Experimental Paper Competition

SKILLS

- **Programming:** Python, C/C++, Java, MATLAB, Mathematica, Latex
- **Software:** VASP, FHI-aims, VESTA, Mathematica, MATLAB, Vim, Material Studio
- **Standard English Test:** TOFEL: 101 (MyBest Score: 108 -- Reading 28, Listening 26, Speaking 27, Writing 27)
  GRE: 150 (Verbal) + 170 (Quantitative) + 3.5 (AW), GRE Physics: 980

LEARDERSHIP & ACTIVITY

- Lead the class to get the **Excellent Class Award** of the Year 2017 and 2018 (top3)
- **2017 4th Prize,** Champion Cup (Soccer Competition for College Teams)