Jiawei Zhan

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Education

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

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

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)

PLUBLICATION

- 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* (Aug 14, 2019 submitted to *Journal: Applied Catalysis B: Environmental*)

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, outperforming all previous algorithm 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_3N_4 Achieving Efficient Visible-Light-Driven CO_2 Reduction**
Advisor: Dr. Jin Zhao *Mar. 2018 – 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
- Numerically calculated the reactions' speed, 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 proved 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**

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 oxygen-doping could decrease Gibbs free energies (ΔG) of a significant step that influences 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

AWARDS

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

SKILLS

- **Programming:** Python, C/C++, MATLAB, Mathematica, Latex
- **Software:** VASP, FHI-aims, VESTA, Mathematica, MATLAB, Vim, Material Studio
- **Standard English Test:** TOFEL: 97(Speaking 27)

LEARDERSHIP & 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)