# **BIN (JAKIE) LIAN**

#### **Undergraduate of Material Physics**

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### **EDUCATION**

Bachelor's degree of Material physics University of Science and Technology of China,(USTC)

**2017.08-2021.06** 

**♀** China · Hefei

School of Chemistry and Material Science

UC Berkeley summer session University of California, Berkeley, (UCB)

## 2019 Summer

 $\mathbf{Q}$  California · Berkeley

- Quantum mechanics Physics.137,A
- Introduction to Analysis Math.104,A

Summer Research

**Brown University** 

**2020.07-2020.11** 

**♀** *Online*·(Due to COVID-19)

- Instructor: Prof.Brenda Rubenstein
- Topic: Using the Machine learning Method to Accelerate the Prediction of the Complex Organic substances' behavior on the alloy

### **HONOR & AWARDS**

Leica Cup-National Metallographic Skills Competition for **College Students** 

- First Prize
- July 2018 -Aug 2018, China, Xi'an

The 15th University Physics Innovation Research Paper Competition(USTC)

- Grand Prize
- September 2020 Dec. 2020,@China,hefei
- Tianjiao Fan, Bin Lian, Hao Wang, Yuliang Chen, The New Fast Light Curing 3D Printing, independently choose and finish project and public an article on Physics Experimentation

### China Undergraduate Physics Tournament(USTC)

- Second Prize
- Oct 2018 March 2019,@China,Hefei
- Members: Shengkai Zhu, Bin lian, Qiyuan Wang, Shasha Xu, Zhuang Qian, focusing on topic of The Lopping Pendulum and Flat Selfassembly.

University of Science and Technology of China Excellent Student Scholarship

- First year college ,@China,Hefei
- Second year college ,@China,Hefei

Elite Scholarship of Institute of Chemistry, Chinese Academy of Sciences

- Elite Scholarship
- Third year college ,@China,Hefei

Excellent Volunteer of "60th anniversary for celebrating the establish of USTC"

• Third year college ,@China,Hefei

# TA EXPERIENCE

# **Quantum Physics for Elite Program**

- 2020 Fall Semester, In English, lead 30 students • Textbook: Modern Quantum Mechanics, J.J. Sakurai & Quantum
- Chemistry, Levine.

# **TECHNICAL SKILLS**

**Programming** 

**Python** 

Wolfram Mathematica Linux

HTML5,CSS

Shell Script

Jupyter notebook

Julia

Matlab

MySQL Web crawler **JAVASCRIPT** 

Experiment section:

Chemical experiment skills Physical experiment skills



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# SOFTWARE SKILLS

For Computing & simulation:

**VASP** 

Quantum Espresso Material studio, CASTEP

Multiwfn

**Atomic Simulation Environment Atomic Machine-learning Package** 

Lammps

Gaussian NAMD

**Comsol Muti-Physics** 



For Modeling:

**VESTA** 

Rhinoceros, Shaper 3D



Some others:

Origin Manim



### **PUBLICATION**

• Tian-jiao FAN, Bin LIAN, Hao WANG, Yi-liang CHEN, ···etc. Exploration of the method of light curing 3D printing technology, Physics Experimentation, DOI:10.19655/j.cnki. 1005-4642.2020.09.001

### IMPORTANT COURSE GRADE

#### **Undergraduate Theoretical**

- Quantum Physics: A
- Solid State Physics: A<sup>+</sup>
- Freshmen Seminar: A<sup>+</sup>
- Appl.of CASTEP/Matrial Studio in Material Computation: A<sup>+</sup>
- Characterization Techniques Of Material: A
- Basic Structure of Solid Material: A
- Materials Synthesis and Processing: A
- Quantum Chemistry: A
- Physical Chemistry I & III A<sup>-</sup>

### **Undergraduate Experiment**

- Chemistry Experiment A
- College Physics Experiment IV(Innovation Exp):A<sup>+</sup>

#### **Graduate Course**

• Computational Material Science: A<sup>-</sup>

# RESEARCH INTEREST

#### **Stochastic Electron Structure**

• Electron structure determined many behaviors of a material, Using the Ab- initio Method unearth the great characteristic of one material and help us do deeper understanding from a more intrinsic way, supporting experiment results, moreover find the law!

#### Machine learning & Deep learning and Chemistry Hybrid area

• Every day numerous data was made from tons of calculations, Data here may mean one configuration's binding energy, but when there are thousands of possible Configurations, It really matters to drug the most important fingerprint from data and help to do one category of prediction fast and well.

#### **Theoretical Chemistry**

• For every step we did in one calculation, there was filled with approximation, From basic Kohn-Sham Equation's  $V[n(\vec{r})]_{unknown}$  to wavefunction's Approximation(like Plane-wave approx.), Pseudopotential, etc., I believe when there is an approx. there is an error. So Could we make it better, not via modifying the parameter, but try to improve the basic theory

# ADVANTAGES

- Teamwork
- Fast self-learning
- Open minded

### IMPORTANT PROJECTS

[class paper][Freshman seminar]Exploring the development of semiconductor

- TIME:2018.1-2018.5
- We focus on how The Moore's law were established and dysfunction, Our group via exhuming the history of the industry behind the law, every key upgrade of the technology and breakthrough in basic theory bringing such prosperity to Semiconductor, finally we analyze the reason for Moore's law s broken from quantum mechanics and the semiconductor physics reasons.

#### [Bin Xiang's group] computational Material Science for 2D Materials

- TIME:2019.4-Present
- Focus on doing the calculation of the system  $Cr_{1.39}Te_2$  's MAE(magnetic anisotropy energy ) to support the experiment result
- Independently rebuild the environment of our cluster and help our group upgrade the VASP to the least version to gain the ability to do Non-linear calculations.
- using the Vasp5.4.4 calc the MAE
- calc path: Non-SOC Relaxiation -> Non-SOC Static calculation ->SOC Calc->Add the MAGMA z-axis and changing the SAXIS( quantisation axis for noncollinear spins)direction  $\theta \in [0, \pi], \phi \in [0, \pi],$  $E_{MAE} = E_{\theta} - E_{easy}$

### [Class Project][Quantum Physics] Stretching Vibrations Of A XY2 Molecule As A Training Project For "Quantum Physics"

- TIME:2019.10-2019.12
- Programming in both Python edition and Wolfram Mathematica edi-
- ullet Calculate the  $H_2S$ 's Energy considering the Pertubation Theory in Hamiltonian for a Morse oscillator: $H = \frac{p^2}{2\mu} + D_e \left(1 - e^{-\alpha r}\right)^2$
- Visualizing via Jmol, python, data deal with Numpy

[Class Paper][Computational Material Science] Machine Learning (and Deep learning)in Material Science-Achieve and Application

- TIME:2019.10-2020.1
- Focus on the development of the method in material science research, collect and learn some basic idea of ML & DL as the datadriving method applied in Material science

# The New Fast Light Curing 3D Printing

- TiME:2019.10-2020.1
- Discuss with my group and rising the idea of 3D printing
- Assemble the experiment instruments and do the test
- Principle: lighting curing depends on the accumulation of the energy of a special wavelength light(depends on the resin) when over the threshold it curing. According to the principle, we made the 3D model using a 2D over-

certain morphology We can determine how deep the color we would use. And using the Rhinoceros to create such 2D animation. printing part directly using a commercial laser projector.

lap projection. By calculating the Energy accumulation for forming a

[Summer Research] Using the machine learning method accelerate the complex Organic substances behavior on alloy surface

- TIME:ING(2020.7-2020.10) • Focus on using a machine learning method to accelerate the predic-
- tion of the iodine organism's binding energy, which can give a direct view for judging whether the bond would be broken easily, to help illustrate the catalytic condition on the CuPd alloy surface. By using Gaussian descriptor extract the Feature vector—(fingerprint) out from the geometry of every atoms in the slab and using neural network doing regression, we make a function  $E = \sum_{i=1}^{N} \hat{E}_i \left( \mathbf{G}_i(\tilde{\mathbf{R}}) \right)$ 
  - $G_i(\tilde{\mathbf{R}})$  is the No.I Feature vector. For using the Atom-centered scheme the model can be modified by adding more data in it. Aiming: using the model trained from a relatively simple organism accelerate much more complex one's calculation