# Yu-Jie Cen (he/him)

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## EDUCATION

**School of Physics and Optoelectronics, South China University Of Technology**

M.S. | Degree in Theoretical Physics (2020.9-2023.6)

B.S. | Degree in Applied Physics (2016.9-2020.6)

## RESEARCH EXPERIENCE

- Mentored by Xiao-Bao, Yang and Yu-Jun, Zhao in the Computational Condensed Matter Physics Group.
- A method for screening ground state candidate structures is proposed to accelerate high-throughput first-principle calculation.
- Improving search efficiency of special quasirandom structures (SQS) in high-entropy alloys by supervised learning.
- Search for the ground state structure of two-dimensional boron monolayers by structural self-assembly methods.

## PUBLICATIONS

- Yu-Jie Cen, Chang-Chun He, Shao-Bin Qiu, Yu-Jun Zhao, and Xiao-Bao Yang, Determining ground states of alloys by a symmetry-based classification, Phys. Rev. Materials 6, L050801 (2022).

## SKILLS

- Experienced in Python and Matlab. Working knowledge of Linux systems/tools.
- Scientific computing and machine learning (ML) expertise for physical science problems. Experienced in parallel computation.
- First-principles calculations experience (VASP), such as Formation Energy, Band, DOS, Elastic Modulus and so on.
- Latex and Markdown.

## FELLOWSHIPS AND AWARDS

Outstanding Graduate student (2020)

School scholarship (2017-2019)

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# TEACHING AND OTHER EXPERIENCE

Administrator of the computing server (approximate 1300 cpu cores) in CCMPG (2021 - now)

Teaching assistant of General physics (2021.9 - 2022.1)

China Undergraduate Physics Tournament (2017-2018)

Dear Prof. Frank Ortmann,

To shortly introduce myself, my name is Yu-Jie Cen, and I am currently pursuing a master's degree at South China University of Technology. I will completed my master's degree with a specialization in computational condensed matter physics in June 2023. With reference to the information listed on the TUM vacancies web page, I am writing to express my interest in the PhD position in Theoretical Chemistry/Condensed Matter Physics.

I have the experience in crystal structure prediction and method development for ground states structures. In my master thesis, I screen the possible ground state candidates from the whole configuration space, based on the interactions model of atom classification model and convex hulls analysis. The core of my works is to design an algorithm to reclassify the structures according to symmetry and calculate the vertex structures in the correlation functions space. The result has been published in Physical Review Materials. More information can see in Phys. Rev. Materials 6, L050801.

Besides, I am interesting in using machine learning to solve physics problems. A well-trained machine learning model may be able to combine the strengths of different structures to predict a new high-performing material. I have experience building a special quasirandom structures (SQS) crystal generator containing many-body interactions in high-entropy alloys based on supervised learning with neural networks model in python. The inverse problem of mapping a feature vector to a crystal structure is a typical NP problem. We fix the lattice cell and randomly generate the crystal structures and feature vectors as training dataset. Using the SQS feature vectors as input for prediction, we get the approximate SQS structures. More information can see in this page https://diroccen.github.io/2022-06/a2.

Another work is about the structural stability of 2D boron plane. Because the valence electrons of boron are 5, the pattern of 2D boron plane is very complicated unlike 2D carbon planar graphite. The boron plane will have vacancy defects based on triangular lattice. There are some generalized rules like 2 vacancies cannot be connected together or the structure will be unstable. Using these rules we assemble the structure just like a jigsaw games. Right now we can assemble a crystal structure which primitive cell has approximately 100 atoms and the energy is pretty close to the lowest energy.

In addition, I have the experience in teamwork to complete a big project. I participated in the SAGAR software developed by our group in Python (http://sagar.compphys.cn/sagar), and I am responsible for the module B2 and B3.

For future plan, I wish I could be an academic after PhD, but I'm also happy to keep other options open. I think this PhD position is the best fit for my academic and career. I am very passionate about gaining physical insight and using computer simulations. I think that my efforts and skills could be quite helpful to what the research topic demands.

If you need any additional information, you can reach me at my phone number (086-15521284374) or E-mail (202020129949@mail.scut.edu.cn). Thank you for your time and consideration.

Sincerely,
Yu-Jie, Cen

# Referees information

**Prof. Xiao-Bao Yang (Mentor)**
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ResearchGate: https://www.researchgate.net/profile/Xiao-Bao-Yang
Research group: Computational Condensed Matter Physics Group

**Prof. Yu-Jun Zhao (Co-Mentor)**
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Research group: Computational Condensed Matter Physics Group