Dear Admissions Committee Members,

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. I'm interesting in the fields of computational physics/materials including first-principles calculations, machine learning, statistical mechanics, etc.

In my master thesis, I study the ground state structures of alloys at the atomic scale which is closely related with the prediction of high performance materials. Based on the interactions model of atom classification model and convex hulls analysis, we screen the possible ground state candidates from the whole configuration space. 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 plans, I wish I could be an academic after PhD, but I'm also happy to keep other options open. MPGC-QM has excellent reasercher in atomistic computer simulations, non-equilibrium dynamics and machine learning, which is fitting with my research interests. I hope I'll be lucky enough to join you. Thank you for your time and consideration.

Sincerely,
Yu-Jie, Cen