PennState
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To Whom It May Concern:

I would like to enthusiastically recommend Congzhou (Mike) Sha to attend the Quantum Computing Workshop. Mike is a student of an elite MD/PhD program at Penn State College of Medicine. Mike performed a rotation project in my laboratory in June of 2019. Although I have been fortunate with students, there is a group among all of my students whose performance was beyond any expectations. Mike impressed me with his perseverance and determination similar to that of the best students in my laboratory. His performance was so impressive that I offered him a position in my laboratory even before he completed his rotation.

Mike is highly intelligent and creative. During his rotation, he worked on computational prediction of the RNA structure from its sequence. RNA molecules play critical roles in living systems, especially in the regulation of gene expression. Not only as a passive carrier of genetic information (mRNA), numerous new roles for RNA have been discovered, and it is now clear that RNA participates in every phase of gene expression. Experimental approaches to determining RNA structure are lagging behind those for protein structure determination. Computational approaches can offer significant help in predicting RNA structures. One approach that we are pursuing is to classify and construct a library of RNA 3D motifs, that are recurrent structural modules essential for many biological functions and RNA folding. In his project, Mike was combining RNA 3D motifs and our RNA 3D structure prediction tool, iFoldRNA, to enhance the prediction accuracy and efficiency. I was very impressed by his motivation, independence, and hard work while he was carrying out these activities. Not surprisingly, his effort paid off and he has built the seed library in one month! He has since joined my laboratory; he developed an advanced machine learning code to predict RNA structures. Currently, he is optimizing the code and will combine it with the design algorithm, which is almost complete, to design the first RNA structure computationally. If he succeeds, which I have little doubt, he would develop the first in the world algorithm for RNA design. His first strides have already resulted in a powerful machine learning based approach capable of predicting small RNA structures (Sha et al., "Predicting 3D RNA structure from solely the nucleotide sequence using Euclidean distance neural networks", BioRxiv (2022) doi: https://doi.org/10.1101/2022.05.16.492153).

Regarding the RNA structure prediction project, I believe it is a perfect topic for Mike. He proved that he is capable of doing research of such complexity, and, in fact, wrote his proposal completely by himself. I believe he is poised to succeed in this project. I have funds to support this work in the laboratory. I am particularly excited about this work and plan to perform experimental validation of Mike's predictions. This way, Mike would be exposed to experimental design and execution.

Apart from his project, Mike actively participated in the journal club and group meetings. He presented several interesting publications. During his stay, he always made many valuable contributions to group discussions.

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Mike has great analytical skills. His communication skills are excellent. His writings are clear and precise. He is quick in grasping the subjects. At a personal level, Mike is disciplined and organized. Mike's creativity is expressed well beyond science: he is an outstanding violinist and a dreamer. He has a passion for knowledge and arts and sees the world through the lens of his passions. His desire to help people by becoming a practicing medical doctor is very laudable and goes beyond what most of us mortals can accomplish. I believe Mike can reach every single goal since all of them are driven by passion.

Mike is extremely curious. During his first year in my laboratory, he offered help with a project, just sponsored by the NSF ACCEL program, which is a prestigious high-risk high reward program stemming from the NSF director. He is helping with his machine learning and artificial intelligence algorithms in designing quantum computers for virtual drug discovery. In this project, he is adapting machine learning algorithms that he developed for RNA to drug discovery on quantum computers. This is an extremely challenging project that connects physicists, chemists, engineers, and computer and data scientists to develop something that nobody dreamed of a couple of years ago (Li et al., "Invited: Drug Discovery Approaches using Quantum Machine Learnin", 58th ACM/IEEE Design Automation Conference (DAC), 1356-1359 (2021) doi: 10.1109/DAC18074.2021.9586268). He has already developed a machine learning approach capable of predicting a docked pose of a drug to a protein, NeuralDock (Sha et al., "NeuralDock: Rapid and conformation-agnostic docking of small molecules", Frontiers in Molecular Biosciences, 9:867241 (2022)).

We are currently working on quantum machine learning methods for drug discovery (NSF 2210963) in collaboration with quantum computing researchers at Penn State. Mike is responsible for developing the classical machine learning approaches to topics in drug discovery and molecular dynamics. For example, our recent preprint "Differentiable rotamer sampling with molecular force fields" (Sha, Wang, and Dokholyan, 2023, doi:10.48550/arXiv.2302.11430) aims to replace molecular dynamics of macromolecules completely with neural network sampling of rotameric conformations. Attending this workshop would enable Mike to implement the transition from classical machine learning for macromolecules to quantum machine learning.

Academically, Mike is extremely strong. Beyond his research excellence, he has been excelling in his classes, taking some of the more advanced-level ones. Not surprisingly, he has received several awards for his excellent academic performance, such as Vagelos Endowed Scholar, Hydra Prize, and Vagelos Science Challenge Award. Notably, his score on a very challenging MCAT test is perfect (100%), which makes him a perfect candidate for any medical school in the country.

In summary, Mike has been an outstanding addition to our group. He is a very bright student and I give him my highest recommendation to attend the Quantum Computing Workshop.

Sincerely yours,

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