

The **A**ppled **M**achine Learning and **M**aterials **M**odeling (**AM3**) Group at NUS-MSE is looking for motivated graduate students to join!

Research Interests:

- Computational modeling of complex materials for renewable energy applications (e.g., Li/Na-ion battery cathodes/electrolytes/interfaces)
- Atomistic simulations with statistical mechanics & first-principles calculations in disordered/amorphous/interfacial systems
- AI for Science: machine learning interatomic potentials, generative models, and reaction networks development & applications

Requirements:

- B.S./M.S. in physics/chemistry/computer science/materials science or related fields
- TOFEL ≥ 85 or IELTS ≥ 6.5 . GPA $\geq 80\%$. GRE is preferred.
- We encourage excellent candidates to apply for Graduate Student Fellowships (several [NUS Student Scholarships](#) are available).

Preferred Qualifications:

- Solid foundation in thermodynamics, statistical mechanics, solid-state physics/chemistry
- Proficiency in one mainstream deep learning framework (e.g., PyTorch, JAX)
- Experience in (atomistic) thermodynamic & kinetic simulations (e.g., Monte Carlo, MD)

What we offer:

- We are a new research group offering hands-on training and opportunities to collaboratively explore exciting research areas.
- Our computational group focuses on both methodological development and applications. We will have close collaborations with experimental researchers.
- As a collaborative team, we encourage our graduate students to thrive in interdisciplinary research environments, find their interests, and develop their careers.

You're welcome to get in touch if you agree with our values:

- Our group is grounded in kindness and we strive to create an inclusive environment.
- We do not tolerate harassment or discrimination in any form.
- We value the importance of methodology development & coding practice.
- We honor contributions from all group members.
- We ask for help and value direct communications (speaking > 20 sentences daily).
- We aim to tackle challenging scientific problems with a positive research mindset.
- We commit to acting with honesty & scientific integrity.

Please send an email to peichenzhong617@gmail.com with (1) your CV and (2) a description of your research topics of interest.

Dr. Zhong will be joining NUS as a Presidential Young Professor (tenure-track assistant professor) in Materials Science starting in 2025 Fall. He is now a BIDMaP Fellow at UC Berkeley.

About: [Dr. Peichen Zhong](#) | [LinkedIn](#) | [Google Scholar](#)

BS in Physics (USTC, 2018), PhD in Materials Science (UC Berkeley, 2023)

