國立清華大學
NATIONAL TSING HUA UNIVERSITY

Colloquium

Department of Engineering and System Science, Institute of Nuclear Engineering and Science, National Tsing Hua University

Architecture and Applications of Machine Learning-Driven Multiscale Computational Simulations

In this talk, the following content will be presented:

In this talk, I will focus on how to build an efficient and accurate machine learning-driven multiscale simulation framework. Its objective is to integrate and optimize simulation methods spanning from atomic-level first principles calculation to large-scale molecular dynamics. This integration facilitates more precise predicting of material properties and accelerates the screening of promising materials with exceptional performance characteristics. Machine learning methods play a pivotal role in this framework, speeding up simulations and maintaining the accuracy and reliability of the results. I will take thermoelectric materials and cathode materials as examples to demonstrate the capability of machine-learning interatomic potentials, which makes calculations feasible and applicable to large-scale systems and extended time scales.

邢正蓉教授

Dr. Cheng-Rong Hsing

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Experience :

- Adjunct Assistant Professor (2019~2022), College of General Studies, Yuan Ze University
- Postdoctoral Fellow (2007~2023), Institute of Atomic and Molecular Sciences, Academia Sinica
- Ph.D. in Department of Physics, National Taiwan University (2006)

Research Areas :

- Computational Materials sciences
- Machine learning in materials science
- First-principles calculations
- Random Structure Searching with Objects
- Molecular dynamics simulation
- Quantum Monte Carlo methods

15:30-17:00, Wednesday, March 6th, 2024

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