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臺灣大學應用力學研究所
演 講 公 告

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講　　題：機器學習原子勢能模型於化學複雜材料之應用

主 持 人： 陳國慶所長

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機器學習原子勢能模型於化學複雜材料之應用

Machine-learning-enabled interatomic potential model applied in chemically complex materials

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Abstract

Chemically complex materials are gaining increasing attentions because of their extraordinary properties in various fields, such as high entropy alloy and complex organometal halide perovskite. To properly model the chemical complexities in the compositional space and the permutational space, large-scale atomistic simulations in massive structure sampling are needed. However, it would be extremely time-consuming and resource-consuming if ab initio quantum mechanics simulations were taken place, whereas the reliable forcefield or the interatomic potential for the classical mechanics simulations may be hard to achieve. To find a new method in modelling the chemically complex material with ab initio accuracy result and classical mechanics time and resource requirements is necessary.

Recently, a new type of interatomic potentials has been introduced. The machine-learning-enabled interatomic potential model is constructed using the machine learning method with a massive materials database generated by ab initio quantum mechanics simulations. The machine learning potential enabled the possibility in discussing large scale atomistic models with ab initio accuracy in relatively efficient time and resource considerations. The machine-learning-enabled interatomic potential model can help scientists quickly filter the structures of chemically complex materials by specific material properties, which traditional simulation methods cannot.