第四屆台灣計算力學會議 October 15-18, 2018

Minisymposium Title

Materials Genome and Informatics approach to accelerate the materials discovery and

design.

Description

The Materials Genome Approach is a novel and powerful materials design strategy,

which combines first principle base materials computation and experimental validations

to discover, design, screen and optimize functional materials. Machine learning (ML) and

data mining (DM) enables the researchers to find the unknown correlation, features, and

materials from the database. In addition, ML as the interatomic force field can

significantly accelerates the speed of molecular dynamics simulation. This

minisymposium aims to discuss the application of MGI, informatics (data science,

machine learning ...), or multi-scale simulation for understanding the fundamental

property of materials, accelerating simulation, exploring new materials, and

characterizing the feature of structure.

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