数学与系统科学研究院

计算数学所学术报告

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报告题目：

Accelerating materials discovery through high-throughput ab initio calculations and data mining

邀请人： 周爱辉 研究员

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上午 10:00-11:00

报告地点： 数学院南楼六层

602 教室

Abstract:

With the progress of supercomputers and simulation codes, ab initio calculations have reached a level of maturity which makes it possible to screen thousands of materials searching for specific simple properties. In this talk, I will present this so-called high-throughput ab initio approach and the recent progress achieved in this framework. More complex properties are, however, still out of reach for this high-throughput ab initio approach. In this framework, I will present how machine learning models can be trained on a combination of ab initio calculations and experimental results to achieve interesting predictions. The potential of these two approaches will be illustrated with the search for transparent conducting materials (TCMs) and materials for optoelectronics.

TCMs are critical to many technologies from solar cells to electronics. However, finding materials that combine the two antagonistic properties of large conductivity and transparency to the visible light can be extremely challenging. Combining different ab initio techniques from density functional theory to many-body perturbation theory, we evaluated thousands of materials in terms of essential TCM properties (e.g., band gap and carrier transport). From these results, we will present interesting new compounds as well as discuss the chemistries likely to form high performance TCMs.

Materials combining both a high refractive index and a wide band gap are of great interest for optoelectronics. However, these two properties are typically described by an inverse correlation with high refractive index appearing in small gap materials and vice versa. Here, we conducted a density-functional perturbation theory calculations on more than 4000 semiconductors (with a special focus on oxides). Our data confirm the general inverse trend between refractive index and band gap but interesting outliers are also identified. We will discuss why certain classes of materials perform better.

欢迎大家参加！