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：

A High-Throughput Computational Search for New Transparent Conducting Oxides and New Thermoelectrics

邀请人： 周爱辉 研究员

报告时间：2017 年 6 月 13 日（周二）

下午 16:00-17:00

报告地点： 数学院南楼二层

202 教室

Abstract:

Nowadays, thousands of novel materials can be generated and screened by their computed properties even before their synthesis. In this way, new chemical spaces can be rapidly explored and experiments can focus experiments on the most promising candidates. In this talk, we will present the potential of such high-throughput calculations for searching for new high-performance transparent conducting oxides (TCOs) and thermoelectrics.

TCOs 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 oxides in terms of essential TCO 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 TCOs. We will also present the results for non-oxide materials, identifying zinc blende boron phosphide as a very promising candidate with an optimal band structure.

Thermoelectrics are promising for addressing energy issues but their exploitation is still hampered by low efficiencies. So far, much improvement has been achieved by reducing the thermal conductivity but less by maximizing the power factor. The latter imposes apparently conflicting requirements on the band structure: a narrow energy distribution and a low effective mass. We will describe an original approach to fulfill both requirements in bulk semiconductors. It exploits the highly directional character of some orbitals to engineer the band structure and produce a type of low-dimensional transport similar to that targeted in nanostructures, while retaining isotropic properties. We will then present an overview and preliminary analysis of thermoelectric properties computed with the BoltzTraP code for more than 48000 inorganic compounds from the Materials Project. Finally, we will focus on a new group of thermoelectric materials which have been discovered by the high-throughput screening and which were also investigated experimentally.

欢迎大家参加！