



## 复旦大学数学科学学院 数学综合报告会

报告题目: **Ab initio materials design through high-throughput and data mining**

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报告时间: 2015-11-20 星期五 9:30-10:30

报告地点: 光华东主楼 1801

**摘要:** Many essential materials properties can nowadays be computed using ab initio methods. When coupled with the exponential rise in computational power available to research groups, this predictive power provides the opportunity for large-scale computational searches for new materials. Tens of thousands of novel materials can be generated and screened by their computed properties even before their synthesis, focusing experiments on the most promising candidates and exploring rapidly new chemical spaces.

We will illustrate this by presenting results from a recent search [1,2] for new high-performance transparent conducting oxides (TCOs). Such materials 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 new interesting compounds as well as discuss the chemistries likely to form high performance TCOs.

[1] G. Hautier, A. Miglio, G. Ceder, G.-M. Rignanese, and X. Gonze, Nat. Commun. 4, 2292 (2013)

<http://dx.doi.org/10.1038/ncomms3292>

[2] G. Hautier, A. Miglio, D. Waroquiers, G.-M. Rignanese, and X. Gonze, Chem. Mater. 26, 5447-5458 (2014)

<http://dx.doi.org/10.1021/cm404079a>

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