

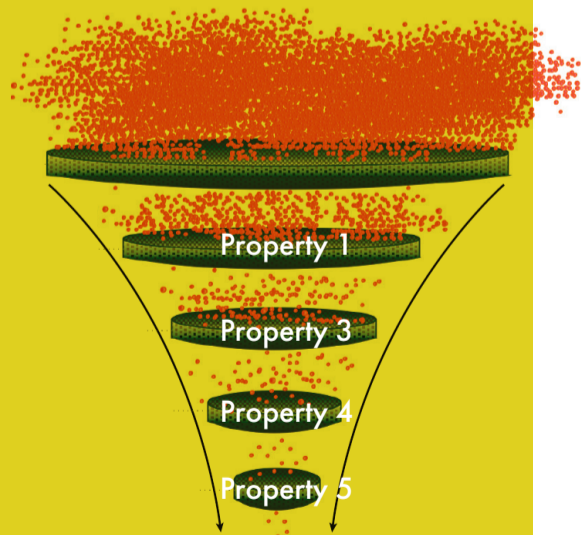
COMPUTATIONAL MATERIALS SCIENCE SEMINAR: SEARCHING FOR MATERIALS WITH EXCEPTIONAL OPTICAL, ELECTRONIC AND SPIN PROPERTIES USING AB INITIO HIGH-THROUGHPUT COMPUTING



Speaker:
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10,000 to 100,000
materials



10 to 100 materials
candidates

ABSTRACT

Essential materials properties can now be assessed through ab initio methods. When coupled with the exponential rise in computational power, this predictive power provides an opportunity for large-scale computational searches for new materials. We can now screen thousands of materials by their computed properties even before the experiments. This computational paradigm allows experimentalists to focus on the most promising candidates, and enable researchers to efficiently and rapidly explore new chemical spaces. In this talk, I will present the challenges and opportunities in materials discovery offered by high-throughput ab initio computing in searching for materials with exceptional optical and electronic properties. Examples from the fields of transparent conducting oxides, electrides and ferromagnetic semiconductors will be especially highlighted. As high-throughput computing generates large amounts of data, I will end my talk by giving an update on the new properties recently added to the Materials Project (www.materialproject.org), including electronic transport but also phonon and vibrational properties.

BIOGRAPHY

Professor Geoffroy Hautier received a Master degree in Materials Science and Engineering from Université Libre de Bruxelles (Belgium) and from Ecole Centrale Paris (France). He obtained his PhD from the Massachusetts Institute of Technology (USA) in 2011 working with Professor Ceder on high-throughput computing for structure prediction and Li-ion battery materials discovery. He joined afterwards the group of Professor Xavier Gonze in Université catholique de Louvain (Belgium) as Marie Curie and FNRS postdoctoral fellow. He focused there on opto-electronic materials and transparent conducting oxides. Geoffroy Hautier is now Associate Professor at the Université catholique de Louvain. He leads a group focusing on computational materials design and high-throughput screening for various applications from photovoltaics to Li-ion batteries (perso.uclouvain.be/geoffroy.hautier/). Professor Hautier is one of the early developer and co-PI of the Materials Project (www.materialsproject.org), a freely accessible high-throughput computational database. He authored more than 90 publications which are cited more than 10 000 times with a h-index of 38. Professor Hautier is an Associate editor for the journal npj computational materials.

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