

## **GEOFFROY HAUTIER**

**Title: “Challenges and opportunities in the high-throughput computational search of new opto-electronic materials”**

### **Abstract**

New opto-electronic devices from solar cells to transparent transistors require high performance materials. Ab initio high-throughput computations offer an accelerated path towards the discovery of these exceptional 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. We will show how simple DFT band structures can be used to screen for promising materials followed up with more expensive theories including many-body or electron-phonon effects. 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 (<http://www.materialproject.org>), including electronic transport but also phonon and vibrational properties.