High-throughput *ab initio* computations for materials design and the Materials Project database

Geoffroy Hautier

Universite Catholique de Louvain

Many essential materials properties can nowadays be computed through *ab initio* methods in the density functional theory (DFT) framework. 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.

In this talk, I will review the challenges and opportunities for *ab initio* high-throughput computing. The problem of finding new inorganic compounds will be addressed and techniques based on data mining which tackle this problem with reasonable computational budget will be presented. To illustrate the benefits of high-throughput computing, I will present results from a computational search of new Li-ion battery cathode materials. Finally, I will introduce the *materials project* : a large publicly available database of materials properties obtained by *ab initio* high-throughput computing (http://www.materialsproject.org).