



United Nations  
Educational, Scientific and  
Cultural Organization



ICTP - East African Institute  
for Fundamental Research  
under the auspices of UNESCO

## **Discovering and Exploring New Materials through the Materials Project**

Anubhav JAIN  
Lawrence Berkeley National Lab, USA

### **Abstract**

The Materials Project was first released in 2011 as a database containing the calculated properties of tens of thousands of materials. Since that time, its database has expanded to >130,000 materials and it has registered over 150,000 users worldwide.

Today, the scope of the Materials Project includes developing interactive tools for exploring the data (e.g., multi-component phase diagrams, Pourbaix diagrams) as well as maintaining an ecosystem of open-source software tools that encompass designing, running, and analyzing the outputs of calculations. These tools have been used to design several experimentally-confirmed materials in a variety of applications, including Li-ion battery cathodes, solid state Li-ion conductors, materials for multivalent batteries, new phosphor materials, and new thermoelectric materials, to name a few. In this talk, I will present an overview of the Materials Project, including its web interface, software tools, and applications.

Next, I will present new capabilities recently researched and being expanded in the near future, such as community contributed data sets through the MPContribs platform which can be used to add experimental data and connect it with the core computational data set.

Finally, I discuss how the availability of and discoverability of these data sets can facilitate the discovery of new critical materials, whether that is through high-throughput screening, stimulating better theoretical method development, or by the application of machine learning methods trained on large data sets.