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ICAMS Seminar

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High-Throughput Computational Search of New Materials and its Application to Lithium-Ion Batteries

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.[1] 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.[2-3] To illustrate the benefits of high-throughput computing, I will present results from a computational search of new Li-ion battery cathode materials.[4-6] Finally, I will introduce the *materials project* : a large publicly available database of high-throughput computing (http://www.materialsgenome.org).

[1] A. Jain et al., “A high-throughput infrastructure for density functional theory calculations,” *Computational Materials Science*, vol. 50, pp. 2295-2310, Apr. 2011.
[2] G. Hautier, C. C. Fischer, A. Jain, T. Mueller, and G. Ceder, “Finding Nature’s Missing Ternary Oxide Compounds Using Machine Learning and Density Functional Theory,” *Chemistry of Materials*, vol. 22, no. 12, pp. 3762-3767, 2010.
[3] G. Hautier, C. Fischer, V. Ehrlacher, A. Jain, and G. Ceder, “Data Mined Ionic Substitutions for the Discovery of New Compounds,” *Inorganic Chemistry*, vol. 50, no. 2, pp. 656-663, 2011.
[4] G. Ceder, G. Hautier, A. Jain, and S. P. Ong, “Recharging lithium battery research with first-principles methods,” *MRS Bulletin*, vol. 36, no. 3, pp. 185-191, 2011.
[5] G. Hautier et al., “Phosphates as Lithium-Ion Battery Cathodes: An Evaluation Based on High-Throughput ab Initio Calculations,” *Chemistry of Materials*, vol. 23, pp. 3945-3508, 2011.
[6] T. Mueller, G. Hautier, A. Jain, and G. Ceder, “Evaluation of tavorite-structured cathode materials for lithium-ion batteries using high-throughput computing,” *Chemistry of Materials*, vol. 23, pp. 3854-3862, 2011.