Poster Session | D. Data-Driven and Physics-Informed Materials Discovery and Design

[PO-D2]Poster Session 2

Symposium D

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-33]Development of First-principles Platform Technology for Energy Research

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As future energy technologies such as high-capacity energy storage and renewable energy applications require exceptional functionalities of host materials, the importance of employing a novel material is getting bigger and bigger. However, discovering a new superior material is very hard to success though it requires large costs and manpower. Recently, many researchers attempt to use an informatics technology such as machine learning in materials screening to overcome the realistic limitations of conventional trial and error method. The key to successive research using informatics technology largely depends on the quantity and quality of the considered database rather than technical details of informatics model. Since property data from experiments are usually sparse or biased to favorable materials in industry, it is hard to obtain a practical database for the informatics research. In that point of view, first-principles calculation is an excellent tool for generating systematic and reliable data of materials properties. However, first-principles calculation itself also requires considerable computational resources and many practical properties are hard to obtain by simple calculations. Therefore, a decent automation of first-principles calculation can do a significant role to establish a successive database. In this talk, I’ll introduce the first-principles platform of Korea Institute of Energy Research aiming at providing a practical computing platform for various researchers with different backgrounds. After introducing the importance of well-defined automation procedure in former materials design studies such finding novel high-k dielectrics and p-type transparent oxides, I'll introduce the automated platform technology for surface-adsorption reactions which have great importance in most energy applications.