Spring 2018 Joint Colloquium
Materials Department & Materials Research Laboratory

Professor Tim Mueller
Dept. of Materials Science and Engineering
Johns Hopkins University

Friday, May 4th, 2018
11:00 am, ESB 1001

The Effective Use of Data in Materials Research

Rapid advances in information technology have made it possible to generate, analyze, and distribute large data sets of material properties. One of the great challenges in materials research is to effectively make use of these data sets to accelerate the design and development of new materials. To this end, I will discuss how data can be leveraged in three ways: 1) I will demonstrate how machine learning can be used to efficiently develop cluster expansions for alloy catalysts that give unique insights into their structure, stability, and catalytic activity. Examples will be drawn from work on platinum alloy surfaces and nanoparticles for the oxygen reduction reaction. 2) I will demonstrate how genetic programming can be used to rapidly identify relevant descriptors for material properties, facilitating rational materials design. 3) I will demonstrate how informatics can be used to rapidly generate highly efficient *k*-point grids, addressing a longstanding problem in computational materials research. Our group has developed a publicly accessible k-point grid server backed by a database of tens of thousands of *k*-point grids, and we estimate that for a broad range of computational methods the use of this server should nearly double the speed of electronic structure calculations on materials.

Bio

Tim Mueller is an Assistant Professor of Materials Science and Engineering at Johns Hopkins University. His research is focused on the use of computational methods to accelerate the design and development of new materials. Prior to joining the faculty of Johns Hopkins in 2012, Tim cofounded Pellion Technologies, a company that is leveraging computational tools to develop advanced batteries. He has an A.B. in Applied Mathematics from Harvard University and a Ph.D. in Materials Science and Engineering from MIT.

http://muellergroup.jhu.edu

Hosted by Anton Van der Ven.