EPFL Valais, ChE 602 Seminar, 02.03.2017

Title: Computational and Data-driven Discovery of Materials

Abstract:
The current state-of-the-art material modeling tools allow for accurate *in silico* prediction of materials properties, and to some extent also prediction of material structures. However, these tools do not typically provide capability to discover structures with the desired properties nor they do guide experimental efforts to synthesize the predicted materials. My work focuses on the development of new discovery approaches, which aim at addressing these challenges. They include similarity-based and optimization-based approaches to materials screening, which require expensive characterization only for carefully selected and statistically relevant subset of a database, therefore enabling discoveries at a minimal computational cost. I do also work on development of databases of predicted material structures, and recently also on synthesizability prediction.

My talk will give an overview of developments in structure enumeration, characterization and high-throughput screening in the context of energy-related applications, and I will demonstrate applications of the developed tools for various classes of materials, including nanoporous materials, ionic liquids and molecular materials.

Bio:
Dr. Maciej Haranczyk received a PhD degree in Chemistry from University of Gdansk in Poland in 2008. During his graduate studies, he spent extended periods at Pacific Northwest National Laboratory, University of Southern California and University of Sheffield. After the graduate school, he moved to Lawrence Berkeley National Laboratory, which had offered him a Glenn T. Seaborg Postdoctoral Fellowship. He was then hired into a Research Scientist position (2010) and subsequently promoted to a Staff Scientist position (2014). In Summer 2015, he joined IMDEA Materials Institute in Madrid as a Senior Researcher, where he leads efforts in the area of computational and data-driven materials discovery.