

EPFL Valais, ChE 602 Seminar, 01.12.2016

Title: The Nanoporous Materials Genome in Action

Abstract:

It is now possible to make an enormous spectrum of different, novel nanoporous materials simply by changing the building blocks in the synthesis of Metal Organic Frameworks (MOF) or related materials. This unique chemical tunability allows us to tailor-make materials that are optimal for a given application. The promise of finding just the right material seems remote however: because of practical limitations we can only ever synthesize, characterize, and test a tiny fraction of all possible materials. To take full advantage of this development, therefore, we need to develop alternative techniques, collectively referred to as Materials Genomics, to rapidly screen large numbers of materials and obtain fundamental insights into the chemical nature of the ideal material for a given application. In this presentation we will show how one can use this approach to find materials for a range of different energy-related applications.

Bio:

Berend Smit received an MSc in Chemical Engineering in 1987 and an MSc in Physics both from the Technical University in Delft (the Netherlands). He received in 1990 cum laude PhD in Chemistry from Utrecht University (the Netherlands). He was a (senior) Research Physicist at Shell Research from 1988-1997, Professor of Computational Chemistry at the University of Amsterdam (the Netherlands) 1997-2007. In 2004 Berend Smit was elected Director of the European Center of Atomic and Molecular Computations (CECAM) Lyon France. Since 2007 he is Professor of Chemical Engineering and Chemistry at U.C. Berkeley and Faculty Chemist at Materials Sciences Division, Lawrence Berkeley National Laboratory. Since 2014 he is director of the Energy Center at EPFL.

Berend Smit's research focuses on the application and development of novel molecular simulation techniques, with emphasis on energy related applications. Together with Daan Frenkel he wrote the textbook *Understanding Molecular Simulations* and together with Jeff Reimer, Curt Oldenburg, and Ian Bourg the textbook *Introduction to Carbon Capture and Sequestration*.