



THE OHIO STATE UNIVERSITY

The William G. Lowrie Department of Chemical and Biomolecular Engineering Graduate Program

Cordially invites you to attend a seminar on

Big-data in Chemical Engineering: Science Beyond Understanding

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Monday, February 14th, 11:30 AM

Zoom Webinar URL:

<https://osu.zoom.us/j/92097483753?pwd=czJ2KzF5bzdt aHZxcml0aEZnMTFpZz09>

Password: 020221

Abstract

Can we tailor-make a material that is optimal for a given separation? The conventional approach is to design the separation process and evaluate the different materials typically used in separations. But what to do if modern chemistry gives us the tools to make millions of materials? With so many materials, we will have a lot of data and modern data-science tools on how to analyze the data. In this presentation, we show how data science can impact the future of chemical engineering. We discuss the challenges of having to deal with thousands of materials. How can we predict the performance of a material in a separation process with a lack of experimental data or even before it has been synthesized? That we have so many materials gives new opportunities to make predictions of properties of materials for which we have no theory. In this presentation, we illustrate how data science methods have helped us learn from a wide range of questions. How can we improve the synthesis of materials by learning from failed experiments? Can we use big-data to design novel materials for separating wet flue gasses? Can we understand the amine emission of a carbon capture plant?

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 Physicists 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. In 2007 he was appointed Professor of Chemical Engineering and Chemistry at U.C. Berkeley and Faculty Chemist at Materials Sciences Division, Lawrence Berkeley National Laboratory.

Since July 2014 he is full professor 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](#).

