

Computational Carbon Capture

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Abstract

The separation of mixtures of volatile molecules presents a critical issue in the clean use of existing fuels and in the generation of alternative fuels. In particular separation of CO₂ is at present one of the mayor barriers for large scale CO₂ sequestration. For example, the conventional technology for capturing CO₂ from the effluent stream of a power plant may require as much as 25% of the electricity being produced. In this presentation an overview will be given on the activities on carbon capture the Energy Frontier Research Center (EFRC) in Berkeley.

In this presentation we describe how computational techniques can be used to screen novel materials for carbon capture. Our starting point is the question how to define the optimal material. We introduce the concept of parasitic energy as a metric to compare different materials; the best material is the material that minimizes the loss of efficiency of a power plant. To compute this parasitic energy one need information on the mixture isotherms of the various components of flue gasses. We show how quantum chemical calculations can be used to predict the adsorption energies. In addition, we show how these calculations can be used to develop a force field that allows us to predict the adsorption properties. We will apply these methods for materials for which experimental data is lacking, or for materials that have not yet been synthesized.

Categories and Subject Descriptors

J.2 Computer Applications, PHYSICAL SCIENCES AND ENGINEERING: Chemistry -- Nouns: SCR

Keywords

Carbon Capture; Materials Genome; Molecular Simulations; nanoporous materials

Short 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 2009 he is the director of the Energy Frontier Research Center for gas separations relevant for clear air technologies.



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*.

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