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SEMINAR SERIES

HIGHLIGHTS IN ENERGY RESEARCH

14.02.2019, 16:00 - 17:00, EPFL Valais, 4th floor, ZEUZIER room

Ab initio free energy calculations for gas adsorption and separation in nanoporous systems

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Host : Prof. Berend Smit

Metal-organic frameworks (MOFs) are promising materials for gas storage, e.g. storage of energy carriers such as H_2, and gas separation processes, e.g. removal of CO_2 from CH_4. The rational design of new adsorbents with enhanced separation performance at optimized separation conditions requires reliable predictions of adsorption isotherms and co-adsorption selectivities with no other input than the atomic position. This we achieve with Grand Canonical Monte Carlo (GCMC) simulations on a lattice of adsorption sites. The Hamiltonian is defined by Gibbs free energies of adsorption on individual sites and lateral interaction energies (adsorbate-adsorbate) calculated, both obtained with quantum chemical *ab initio* calculations.
Currently, co-adsorption isotherms are almost exclusively obtained from single component isotherms using the Ideal Adsorbed Solution Theory (IAST). Based on our ab initio calculation we analyse the underlying approximations and propose an improved model for systems with strong lateral interactions.

CV: Prof. Joachim Sauer
Joachim Sauer received the Dr. rer. nat. degree in Chemistry from Humboldt University in Berlin in 1974, and the Dr. sc. nat. degree from the Academy of Sciences in (East-)Berlin in 1985. Since 1993 he was Professor of Theoretical Chemistry at the Humboldt University in Berlin, and since 2006 external member of the Fritz Haber Institute (Max Planck Society). He is member of the Berlin-Brandenburg (formerly Prussian) Academy of Sciences, the German National Academy Leopoldina, and foreign member of the Royal Society. He is one of the editors of the Journal of Catalysis. His research has explored the application of quantum chemical methods in chemistry, with emphasis on surface science, particularly adsorption and catalysis. He has published more than 380 research papers, notably in the area of modeling the structure and reactivity of transition metal oxide catalysts, zeolites and metal-organic frameworks, and he has given more than 475 invited lectures. He was awarded with the Francis Gault Lectureship of the Federation of European Catalysis Societies (EFCATS) and the Schrödinger medal of the World Association of Theoretical and Computational Chemists (WATOC).