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CHEMICAL AND BIOLOGICAL ENGINEERING

SEMINAR ANNOUNCEMENT

DR. J. ILJA SIEPMANN

"Predictive Modeling of Adsorption and Transport in Nanoporous Materials: From High-Throughput Screening to First Principles Simulations"

Dr. J. Ilja Siepmann
Distinguished McKnight University Professor, a Distinguished Teaching Professor, and member of the graduate faculties in chemistry, chemical physics, chemical engineering, and materials science at the University of Minnesota

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Abstract

Nanoporous materials, such as zeolites and metal-organic frameworks, play numerous important roles in modern oil and gas refineries and have the potential to advance the production of fuels and chemical feedstocks from renewable resources. The performance of a nanoporous material as separation medium and catalyst depends on its framework structure and the type or location of active sites. To date, more than 200 zeolite framework types have been synthesized and more than 330000 thermodynamically accessible zeolite structures have been predicted, and the corresponding numbers are significantly larger for metal-organic frameworks. Hence, identification of optimal nanoporous materials for a given application from the large pool of candidate structures is attractive for accelerating the pace of materials discovery. Here we identify, through a large-scale, multi-step computational screening process, promising nanoporous materials for (i) purification of ethanol from fermentation broths, (ii) sweetening of highly sour natural gas mixtures, and (iii) hydroisomerization of linear to slightly branched alkanes with 18-30 carbon atoms. This talk will also highlight recent developments enabling first principles Monte Carlo (FPMC) simulations for which the potential energy is calculated on-the-fly using Kohn-Sham density functional theory. Applications of FPMC to the prediction of (a) adsorption isotherms for gas molecules in metal-organic frameworks with under-coordinated metal nodes and (b) reaction equilibria in cation-exchanged zeolites. Emphasis will be given to simulation methodologies and microscopic-level origins of the observed thermodynamic behavior.