Discovery of optimal zeolites for challenging separations and chemical conversions through predictive materials modeling[1] J. ILJA SIEPMANN, PENG BAI, MICHAEL TSAPATSIS, University of Minnesota, CHRIS KNIGHT, Argonne National Laboratory, MICHAEL W. DEEM, Rice University — Zeolites play numerous important roles in modern petroleum refineries and have the potential to advance the production of fuels and chemical feedstocks from renewable resources. The performance of a zeolite as separation medium and catalyst depends on its framework structure and the type or location of active sites. To date, 213 framework types have been synthesized and ¿330000 thermodynamically accessible zeolite structures have been predicted. Hence, identification of optimal zeolites 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 zeolite structures for two energy-related applications: the purification of ethanol beyond the ethanol/water azeotropic concentration in a single separation step from fermentation broths and the hydroisomerization of alkanes with 18-30 carbon atoms encountered in petroleum refining. These results demonstrate that predictive modeling and data-driven science can now be applied to solve some of the most challenging separation problems involving highly non-ideal mixtures and highly articulated compounds.

J. Ilja Siepmann
University of Minnesota

Date submitted: 12 Nov 2014   Electronic form version 1.4