Predictive Materials Modeling for Energy Systems: Discovery of Optimal Zeolites for Ethanol/Water Separation and Alkane Hydroisomerization

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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: (i) with the ability to purify ethanol beyond the ethanol/water azeotropic concentration in a single separation step from fermentation broths and (ii) with up to two orders of magnitude better adsorption capability than current technology for linear and slightly branched 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.