Program in Polymers and Soft Matter

SEMINAR

"Novel Polymer Membranes for Critical Gas Separations"

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Polymeric membranes, which present an efficient solution for emergent technologies, such as CO_2 capture and natural gas purification, are effective at the selective and efficient transport of gases. The field of polymer membrane design is primarily based on empirical observation, which limits the discovery of new, advanced materials most appropriate for separating a given gas pair. Instead of relying on exhaustive experimental investigations, we apply machine learning on a limited set of experimental gas permeability data for six different gases in ~700 polymeric constructs that have been measured to date to predict the behavior of over 10,000 homopolymer architectures that are currently known. We use a topological, path-based hash of the polymer repeating unit to identify candidates that are predicted to have superior performance. We have synthesized and tested two of the most promising materials identified by this approach and we find that they perform better for CO_2/CH_4 separations than any other polymers tested to date. This machine learning technique, which only uses a small body of experimental data (and no simulation data) to accurately predict the behavior of large classes of polymers, evidently represents a novel means of exploring the vast phase space available for polymer membrane design in a manner that is orders of magnitude more efficient than typical empirical observations.

In a second vein we develop novel membranes based on polymer-grafted nanoparticles (GNPs) which possess controllable, spatially inhomogeneous gas transport behavior. We show that smaller gases are transported more uniformly than larger solutes in the polymer layer of pure GNPs; these larger gases preferentially move through the interstices between the NPs. Free chains added to these GNPs preferentially segregate into these interstices where they selectively hinder large solute motion and thus yield dramatic performance improvements for several industrially relevant gas pairs. The magnitude of these effects are controlled by grafting parameters and the length of the free chains. Our ability to create and tune spatial inhomogeneities in GNPs, apparently through judicious manipulation of chain entropy, is thus a new, apparently general, physics-based paradigm to design membranes with unprecedented performance even using common polymers.