Molecular Scale Engineering of New Materials for Energy-Efficient Separations

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Controlling the chemical and morphological structure of polymers and porous materials has dramatic implications on molecular transport within these materials. Therefore, by properly designing new materials, previously unattainable property sets can be achieved for molecule separations. From a practical point of view, such molecular scale engineering is necessary to identify new, environmentally benign, and more energy-efficient separation technologies than those currently practiced. In the U.S., more than 40,000 distillation columns perform more than 200 separations, which accounts for 49% of industrial separation energy consumption. In addition to distillation, environmentally harmful processes such as amine absorption are currently used on very large scales, so a pressing need exists to identify alternatives to these separation technologies. Of particular promise are membrane-based separations, which, unlike distillation, circumvent the enthalpic energy penalty required for phase changes, and, unlike absorption, operate under steady-state conditions without the need for regeneration. Here, three strategies are presented for designing new membrane materials for enhanced separation performance. First, diffusion-selective polymers known as thermally rearranged polymers and second, solubility-selective perfluoropolymers are considered. The mechanism of gas transport in these materials is investigated from the fundamental perspective of gas-polymer interactions and the creation of diffusional pathways for selective transport of small molecules. Third, an alternative approach to improving membrane performance is presented, whereby highly efficient metal-organic frameworks (MOFs) with outstanding adsorption-selectivities are dispersed into polymers matrixes. This final strategy leverages the processability of polymers and the separation performance of MOFs to form composite membranes with property sets far beyond those achievable with polymers alone.