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Molecular Engineering of High-Performance Nanofiltration Membranes from Intrinsically Microporous Poly (Ether-Ether-Ketone)

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Abstract : Poly(ether-ether-ketone) (PEEK) has received increased attention due to its outstanding performance in different membrane applications including gas and liquid separation. However, it suffers from a semi-crystalline morphology, bad solubility and low porosity. To fabricate membranes from PEEK, the usage of harsh acid such as sulfuric acid is essential, regardless its hazardous properties. In this work, we report the molecular design of poly(ether-ether-ketones) (iPEEKs) with intrinsic porosity character, by incorporating kinked units into PEEK backbone such as spirobisindane, Tröger's base, and triptycene. The porous polymers were used to fabricate stable membranes for organic solvent nanofiltration application. To better understand the mechanism, we conducted molecular dynamics simulations to evaluate the possible interactions between the polymers and the solvents. Notable enhancement in separation performance was observed confirming the importance of molecular engineering of high-performance polymers. The iPEEKs demonstrated good solubility in polar aprotic solvents, a high surface area of 205–250 $m^2\ g^{-1}$, and excellent thermal stability. Mechanically flexible nanofiltration membranes were prepared from N-methyl-2-pyrrolidone dope solution at iPEEK concentrations of 19–35 wt%. The molecular weight cutoff of the membranes was fine-tuned in the range of 450–845 g mol^{-1} displaying 2–6 fold higher permeance (3.57–11.09 L $m^{-2}\ h^{-1}\ bar^{-1}$) than previous reports. The long-term stabilities were demonstrated by a 7 day continuous cross-flow filtration.

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