
DEMONSTRATING THE POTENTIAL OF MOLECULAR-LEVEL ENGINEERING FOR THE PREPARATION OF HIGHLY EFFICIENT COMPOSITE MATERIALS FOR TARGETED GAS SEPARATIONS

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Since 2020, our research group has been developing an innovative molecular engineering (MLE) concept for the fabrication of efficient mixed matrix membranes (MMM) for gas separation with targeted nanoparticles. The concept enables precise control of additive properties and their deposition, thereby eliminating the common weaknesses of material MMMs, such as randomness, phase separation, aggregation, and additive sedimentation. In general, MLE enables the targeted development of nanostructured MMMs for fabricating highly efficient membrane separation materials with tailored morphology and surface properties.

In the initial phase, we developed multifunctional magnetic nanoparticles (SMNPs) from metal-organic framework (MOF) UiO-66, decorated with $\text{Co}_{0.5}\text{Ni}_{0.5}\text{FeCrO}_4$ spinels, which were directly grown on oxidized single-walled carbon nanotubes (SWCNTs) and graphene oxide (GO) monolayers [1]. Subsequently, a single-crystal magnetically responsive core-shell MOF UiO-66-NH₂ grafted with magnetic nanoparticles was prepared and exhibited magnetic-stimulus-responsive behavior. This material was used for controlled deposition in polymethyl methacrylate (PMMA)-based MMMs. The controlled deposition of the MOF yielded excellent permeability and H₂/CO₂ selectivity, exceeding the Robeson upper limit of 2008 compared to PMMA+MOF MMMs without controlled magnetic deposition [2]. We further synthesized a channel layer of zeolite-imidazole framework (ZIF-8) nanoparticles on a free-standing, chemically modified single-walled carbon nanotube (SWCNT) membrane via chemical bonding. The SWCNT-ZIF-8 composite support was sprayed with a thick hydrophobic PDMS layer, and the resulting composite membrane exhibited improved mechanical and thermal stability, as well as excellent performance in CO₂/N₂ gas separation and C₃ olefin/paraffin vapor separation. [3]

Another example is the multifunctional 2D-MXene-based nanocomposite, in which CoFe₂O₄ nanoparticles are grafted onto Ti₃C₂T_x sheets and aligned in a polyethersulfone (PES) matrix via magnetic-field-assisted deposition. The resulting films synergistically combine structural organization with high stability, magnetic sensitivity, and exceptional sorption capacity. In addition, the material exhibits excellent gas separation performance, with an O₂ permeability of 67 Barrer and an O₂/N₂ selectivity of 11.5, which exceeds the upper limit of Robeson theory across the temperature range from 298 to 350 K and at inlet pressures of 0.1 to 2 bar. [4]

In addition to the above examples, the lecture will present further examples demonstrating the MLE concept's ability to prepare highly efficient MMM separation materials from common polymers and with minimal nanoparticle content (< 10 wt.%). The above findings underscore the potential of the MLE concept to achieve simultaneous increases in permeability and selectivity for various gas pairs, thereby moving to the upper-right corner of the Robeson diagrams and potentially guaranteeing both performance and cost for successful use in industrial applications.

Keywords: Gas separation, Mixed matrix membranes, Molecular engineering, O₂/N₂ separation, Magnetic field, Chemical bonding, gas sorption

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