

**Polymer Membranes and Nanostructured Materials:  
AI/ML in Advanced Manufacturing, Characterization, and Self-Driving Labs**

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# ABSTRACT

Membrane and separations technology is a driving force for both fundamental and applied research that impacts the economy. Polymer materials are a vast design space that can be further exploited towards high-performance membrane and filtration applications. Machine learning (ML) can be used to improve membrane materials and design using datasets and data analytics with agentic AI tasks from large language models (LLM). The applications of AI/ML workflows include membrane polymer structure-composition-processing-property (SCPP) relationships, membrane testing, and performance validation. Characterization methods to quantify transport, permeance, selectivity, and environmental stability of membranes need to go beyond statistical methods. Generative AI workflows are important for science discovery and rapid feedback. Exploring bio-inspired designs – de novo membrane design, and future directions will depend on how fast we can implement these workflows. By designing and updating research end-to-end, it is possible to leverage the new tools and datasets becoming available to the membrane community.

## 1. Introduction

The raw materials and chemical needs of modern society are based on extraction or harvesting, conversion or production, and transport or storage systems.<sup>1-3</sup> Energy and material demand from minerals, fossil fuels, and biomass must be balanced at each step with technological, economic, and environmental considerations; hence, the need to understand life-cycle analysis (LCA), techno-economic analysis (TEA), and limited-resource or geopolitical considerations.<sup>4</sup> Separations and purification technologies are highly relevant, especially if they leverage energy savings or minimize heat loss. About 10-15% of the world's energy consumption is for extraction and separations from raw materials. An interesting article by Sholl et al. focused on seven chemical separations of high global importance, including the separation of hydrocarbons from oil, uranium from seawater, and rare-earth metals from ores.<sup>2</sup>

Membrane and separation technology has emerged as an effective alternative to distillation, cracking, centrifuge enrichment, and seawater desalination, etc.<sup>3,5,6</sup> The advantage is in high efficiency, less capital, energy savings, and scalability.<sup>1</sup> Porous open-cell materials and molecular-level mass transport optimization favor membrane and filtration technologies. Nanofiltration (NF) is preferred for ultimate selectivity, but high energy costs should be balanced with permeability and reduced intrusion pressures.<sup>7</sup> Reverse osmosis (RO) and electrodialysis are important desalination methods that can reduce energy consumption and costs while providing convenient, safe water purification.<sup>5</sup> However, most research and technology development methods are closer to trial-and-error approaches or, at best, to using Taguchi or design of experiments (DOE) methods.

Polymeric materials and composites are 21<sup>st</sup>-century materials.<sup>8</sup> They are mostly deployed due to a wide range of materials and manufacturing methods, mechanical durability, and chemical stability. Advanced manufacturing methods based on engineering thermoplastics and thermosets enable the production of multifunctional membranes. They can be optimized to have a

high-permeability or selectivity trade-off. The classic Robeson plot of selectivity versus permeability in gas separations encompasses about 500 polymers, highlighting the wide range of available polymers.(Figure 1) This does not necessarily include additives, fillers, and nanofillers that make up the final membrane materials and compositions used in commercial applications. High-performance polymers (HPP) for membrane separation are also of high interest, especially for applications in extreme environments.<sup>3</sup>

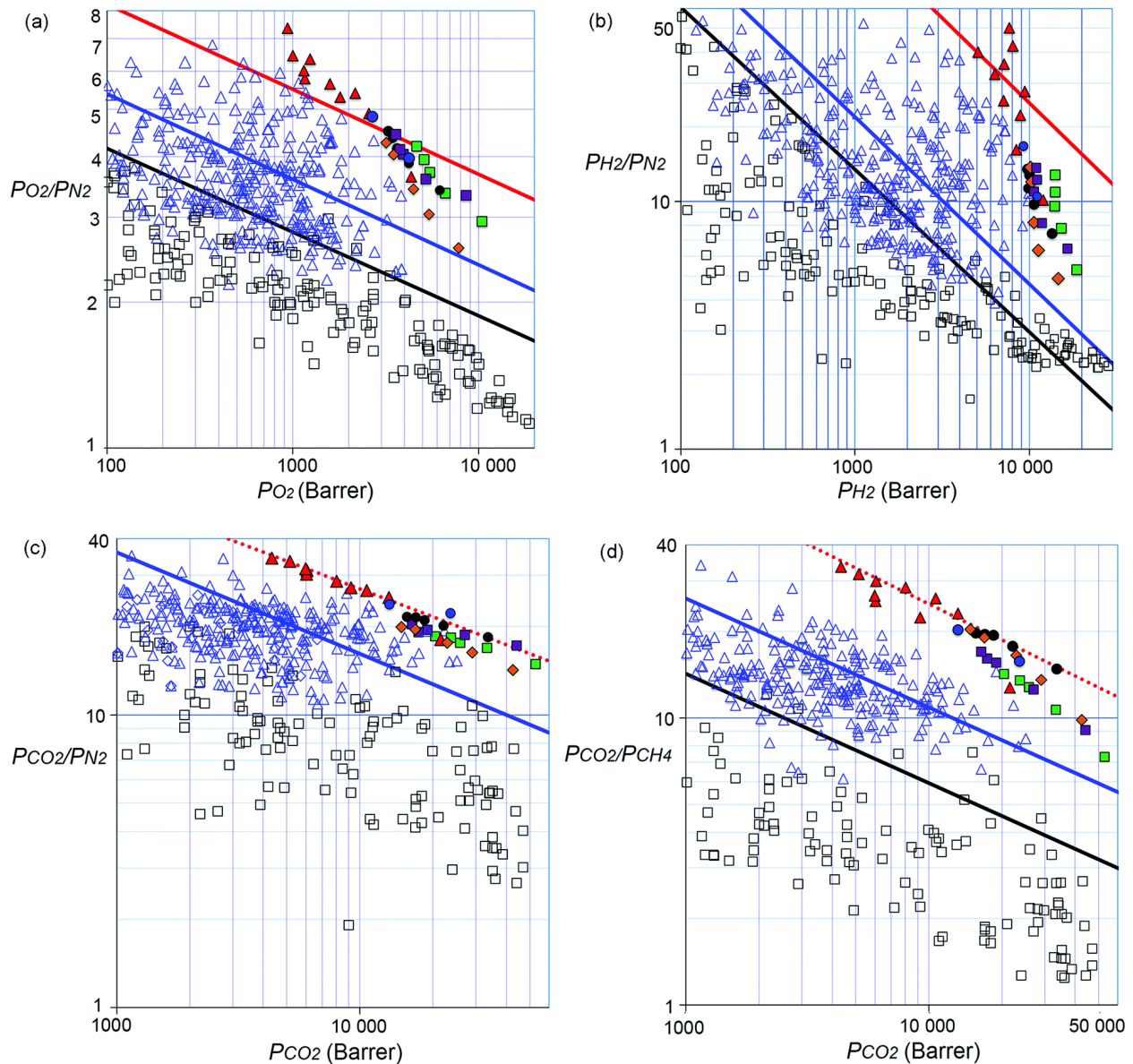


Figure 1. Robeson plots for the (a)  $O_2/N_2$ , (b)  $H_2/N_2$ , (c)  $CO_2/N_2$ , and (d)  $CO_2/CH_4$  gas pairs showing the position of the gas permeability data for films of PIM-BTrip (  $\blacktriangle$  ), PIM-TMN-Trip (  $\blacksquare$  ), PIM-HMI-Trip (  $\blacksquare$  ), PIM-DM-BTrip (  $\bullet$  ), PIM-TFM-BTrip (  $\bullet$  ) and PIM-DTFM-BTrip (  $\blacklozenge$  ). Previously reported data are also shown for non-PIM polymers (  $\square$  ) and PIMs (  $\triangle$  ). Upper bounds are represented by black lines (1991), blue lines (2008), and red lines for the previously proposed (2015) upper bounds for  $O_2/N_2$  and  $H_2/N_2$ . The proposed revised upper bounds for  $CO_2/N_2$  and  $CO_2/CH_4$  are shown as dotted red lines. (Figure and caption from reference<sup>9</sup> with no change under a creative commons 3.0 license<sup>10</sup>)

Investigating the structure-composition-process-property (SCPP) relationships of these polymers and composites, and balancing this trade-off, can be complicated. It is important to have a good understanding of the physico-chemical relationships within these complex material systems. Intrinsic and extrinsic properties accompany the molecular and nanoscopic design up to the macroscopic form factor with fabrication. An alternative to the iterative trial-and-error process is needed and applied to end-to-end process optimization.

Although there are many known and used polymers for membranes (engineering thermoplastics, high-performance polymers, thermosets, etc.) new polymers and composites can still be introduced.<sup>11,12</sup> This is especially true with advanced manufacturing methods, including multilayer co-extrusion, plastisol molding, 3D printing, and co-axial pultrusion. Improved efficiency, performance, and environmental sustainability are driving the need for novel polymers and membrane applications.<sup>13</sup> This includes optimizing parameters such as flux, permeance, permeability, and selectivity for new applications. But the barrier to the synthesis of new polymers and their commercial production can only be justified by the right performance and unit cost ratio, especially with new production line investments. The DOE and other statistical methods are useful for experimental design and membrane development. It can still be accelerated by effective simulation and increasing the rates of formulation, screening, and testing.

There are three main models based on the chemical potential gradient that drives flow and separation: the pore-flow model (liquids), Knudsen diffusion (gases), and solution diffusion model.<sup>1,6,14-17</sup> The Darcy equation provides a first measure of the transport behavior in a porous membrane and is highly empirical:

$$q = kA\Delta P/\mu L \quad \text{eqn 1,}$$

where A is cross-sectional area in cm<sup>2</sup>, k is permeability in Darcy, L is for length in cm, P is for pressure in atm, q is the flow rate in cm<sup>3</sup>/sec, and  $\mu$  is fluid viscosity in cp.

The Knudsen equation describes gas flow in a tube in free-molecular flow. It is expressed by the molecules' mean free path. For gases, depending on the tube diameter, the molecules interact with the walls rather than with each other.

$$q = \Delta P d^3 \sqrt{(2\pi)/(6l\sqrt{\rho_1})} \quad \text{eqn 2,}$$

where q is volume flow rate under unit pressure,  $\Delta P$  is pressure change from the starting point of the tube to the final point, d is for the tube diameter, l is the tube length, and  $\rho_1$  is the density-to-pressure ratio.

Other equations include the Fickian diffusion transport equation and the separation factor in pervaporation methods.

For molecular and macromolecular simulations, first-principles-based design, atomistic-to-coarse-grained methods, and computational simulation tools, including molecular dynamics (MD), density functional theory (DFT), and quantum-chemical methods, can be used.<sup>18,19</sup> They have shown strong potential for predicting material structures and performance. They require high computational costs, and are limited to simpler compositions or conditions, making it harder

to accommodate nanocomposites and new additive packages. Finite element analysis (FEA) methods and other multiphysics simulations are increasingly important for the thermo-mechanical properties of the final membrane and for transport modeling.<sup>20,21</sup> Process simulators are key to modeling, simulating, and optimizing the separation processes in unit operations.<sup>14</sup> The membrane design space can be much wider, with higher throughput, for designing novel membrane materials and optimal fabrication conditions, even across computational and experimental needs.

Artificial intelligence (AI) and machine learning (ML) can accelerate the design, synthesis, and testing or discovery of new cost-effective membranes.<sup>22</sup> ML enables algorithms that leverage data (trained or untrained) to make decisions and predictions. As a complement to conventional computational and experimental approaches, it can be designed to analyze complex data patterns and to develop feedback-loop methods (supervised or unsupervised) for continuous improvement toward ideal data. It can be applied to polymer co-design, composite additive selection, and mechanistic insights into separations, and can be guided towards applications. It relies on high-quality data, which drives the need for effective large language models (LLMs) that are featurized and converted into strong agentic AI tasks.<sup>23,24</sup> ML-driven tools can overcome many shortcomings in the current R&D ecosystem. Our recent reviews and perspectives emphasize the use of AI/ML in future research and discovery science in many materials systems: polymer materials, electronics, bio-based materials, etc., and not just for drug discovery.<sup>25-29</sup> Optimization from existing data and automation of tasks, including agentic AI with LLMs as a backdrop, is the future of materials innovation.<sup>25-30</sup>

Generative AI and deep learning (DL) design could enable more efficient permeation and diffusion control through bioinspired polymer materials and membranes.<sup>31,32</sup> For new materials, there is potential to use 2D nanomaterials, molecular organic frameworks (MOFs)s, covalent organic frameworks (COFs), zeolites, and other inorganic or ceramic hybrids. Combined with polymers, they can improve separation efficiencies and multifunctionality.<sup>33</sup> ML-directed discovery, guided by inverse design principles and nano-, meso-, and micro-scale features, porosity, morphological, and separation-process figures of merit, can enable new discoveries in membrane science. An additional possibility is localized permeabilities, or very low permeabilities, in new polymers<sup>34</sup> which are important for coatings and packaging.

Another use is high-throughput ML-directed validation of the design, with synthesis and membrane testing for fast training, dataset creation, and standards qualification.<sup>22,33,35</sup> An ML-driven virtuous-cycle feedback loop experiment can be realized through an autonomous self-driving lab (SDL). AI/ML will accelerate the timeline from discovery to validation for new membrane systems by enabling rapid screening and manufacturing optimization. By narrowing down optimal materials and processing methods *a priori* through inverse design, this approach reduces the time and resources typically required for extensive experimental iterations. The ML approach has been demonstrated in new polymeric membranes and in the optimization of gas separation, solvent purification, nanofiltration (NF), and pervaporation.<sup>35</sup> Lastly, it can be applied widely to environmental safety, maintenance methods, and operational stability. An end-to-end AI/ML workflow demonstration for the whole membrane ecosystem will be a game-changer. ML algorithms for materials development can predict degradation and anti-fouling properties,

enabling proactive maintenance with increasing membrane sustainability. AI can be used to optimize surface treatment, backwashing cycles, fouling monitoring, chemical cleaning, and energy consumption, thereby adding more operation efficiency.<sup>36</sup> In summary, with scale-up in production and advanced manufacturing, these new material systems can be adopted quickly for new designs and separation geometries in new applications, guided by AI/ML workflows.

## 2. Classification of polymer materials for membranes:

Many polymers are selected based on performance-cost trade-offs as candidates for new membranes and filtration materials.<sup>3,16,37</sup> Polymer choices can be thermoplastics, thermosets, and elastomers. From plastics, they are valued as commodities, engineering, and high-performance polymers, or HPP, using many routes for synthesis.<sup>38</sup> The engineering polymers are a starting point for many membrane materials, but performance in extreme conditions, or higher pressures or temperatures, requires HPPs. For thermoset resins, the combination of more rubbery or elastomeric properties is based on their mechanical properties and processability. Composites and nanocomposites are also good candidates for membranes, improving their functionality for specific applications.<sup>39</sup> The final membrane material is often a formulated additive package that undergoes multiple extrusion or curing stages.

Typical membrane and filtration polymers include: Polysulfone (PSU), Polyethersulfone (PES), polyvinylidene fluoride (PVDF), polytetrafluoroethylene (PTFE), polyimide (PI), polyphenyleneoxide (PPO), polyvinylalcohol (PVOH), polyethylene (PE), polypropylene (PP), Polyacrylonitrile (PAN), silicone, and polyurethane (PU).<sup>3,16,37</sup> Other synthetic polymers are considered PIMs (polymers of intrinsic microporosity). Natural polymers, such as cellulose derivatives and marine-based polysaccharides, are available. These polymers are used to create semi-permeable barriers for filtration and separation in water treatment, medical devices (e.g., hemodialysis), and gas separation. Materials are chosen for their chemical stability, tunable pore structures, and processability, enabling tailored performance across diverse applications.<sup>40</sup> Some typical polymers and their applications are listed below and in Table 1:

- a) PSU and PES: Widely used for water purification due to good chemical and thermal stability, with applications in ultrafiltration.
- b) PVDF: Known for chemical resistance, hydrophobic nature, and use in microfiltration.
- c) PP and PE: Common, cost-effective options for various filtration needs and non-wovens.
- d) PTFE: Highly chemically resistant, often used in harsh environments or challenging solvents.
- e) PI and PPO: Excellent for high-temperature applications and gas separation.
- f) PAN: Versatile, used in water treatment and as a precursor for carbon membranes.
- g) Silicone and PVOH: pervaporation membranes, gas membranes, and high selectivity

Table 1. Applications of common membrane materials <sup>1,6,11,38,39,41-43</sup>

Membrane Material	Micro filtration (MF)	Ultra filtration (UF)	Nano filtration (NF)	Dialysis	Per-vaporation	Gas Separation
Cellulose regenerated	Lab filtration	Protein separation	—	Hemo dialysis	—	—
Cellulose nitrate	Sterilization	DNA/RNA recovery	—	—	—	—
Cellulose acetate	Water treatment	Wastewater	Desalination	Hemo dialysis	—	Yes
Polyamide	—	Support layers	Water softening	—	Organics	Yes
Polysulfone	Pre-filtration	Blood plasma	Support layers	Hemo dialysis	—	—
Poly(ether sulfone)	Food & Beverage	Viral clearance	—	Hemo dialysis	—	—
Polycarbonate	Track-etch filters	Cytology	—	—	—	—
Poly(ether imide)	—	High-temp UF	—	—	—	Yes
Poly(2,6-dimethyl-1,4-phenylene oxide)	—	—	—	—	—	Yes
Polyimide	—	Solvent recovery	Organic NF	—	De-hydration	Yes
PVDF	Oily wastewater	Bio-processing	—	—	—	—
PTFE	Aggressive chems	Membrane dist.	—	—	—	Yes
Polypropylene	Industrial waste	Oxygenators	—	—	—	Yes

Poly-acrylonitrile	—	Enzyme recovery	—	Hemo dialysis	—	—
PMMA	—	—	—	Blood purification	—	—
Poly(vinyl alcohol)	—	—	Metal recovery	—	De-hydration	—
PDMS	—	—	—	—	VOC removal	Bio-gas upgrade

With the growing interest in biobased materials and renewable biomass-based production, natural polymers have gained popularity.<sup>44</sup> Most of these are derived from lignocellulosic or marine-harvested polysaccharides:

- a) Cellulose Acetate (CA) and nitrocellulose (CN) for reverse osmosis and early filtration.
- b) Other cellulose Derivatives: hydroxyethylcellulose (HEC), Hydroxypropyl Methylcellulose (HPMC): are often used for specialized filters and healthcare applications. Also, for sustainable membrane development.<sup>41</sup>
- c) Chitosan, alginate, hydrogels – Filters, additive enhancers, viscosity modifiers, biocompatible, non-allergenic – biomedical applications.
- d) Proteins, silk, and keratins are harvested and processed as fibers and employed mainly for filtration media.
- e) Polylactic acid (PLA): a biodegradable and 3D printable membrane.<sup>45,46</sup>

Polymer properties, including semi-crystallinity, thermo-mechanical properties, pore size, hydrophilicity/hydrophobicity, and surface chemistry, must be controlled during fabrication (e.g., phase inversion, electrospinning).<sup>3,16,37</sup> These polymers are applicable for microfiltration, ultrafiltration, nanofiltration, gas separation, and oil-water separation.<sup>37</sup> Generally, they are lower-cost and easier to manufacture at scale than inorganic and ceramic membranes. Certain polymers are suitable for biomedical applications, such as hemodialysis.

Nanomaterials such as graphene, carbon nanotubes (CNTs), nanoclays, and metal-organic frameworks (MOFs) can be added to form nanocomposite membranes.<sup>47,48</sup> Hydrogels are interesting materials for membranes because of their swelling behavior, as well as their ion-transport and small-molecule transport properties.<sup>49</sup> They are based on synthetic and natural polymers that can be both physically and chemically crosslinked.<sup>50</sup> Indirect metal 3D printing with biobased hydrogel inks was reported, which can be an important method for hybrid-membrane and filter fabrication.<sup>51</sup>

### 3. Methods of Processing and Fabrication of Membranes

Manufacturing methods can be classified as formative, subtractive, additive, or hybrid manufacturing (FM, SM, AM, and HM, respectively), with or without solvent (Figure 2). Molding (including injection molding and reaction injection molding), pultrusion, thermo- or vacuum forming, etc., are all FM methods. The membrane materials for any of these methods require the creation of diffusive (molecular) and porous (micro to milli-) structures for separation. The inclusion of porogens, thermo-chemical treatments, and interfacial polymerizations can generate molecular-level porosity.<sup>52</sup> Often, the diffusion properties are attributed to the molecular and morphological order of the materials (amorphous, semi-crystallinity or cross-linking order). For more macroscopic porosity, this is primarily achieved with phase inversion (NIPS/VIPS for solvent exchange)<sup>53</sup>, melt or electrospinning (fiber formation via heat or electric field),<sup>54</sup> stretching (pore creation by mechanical pulling), track etching (ion bombardment for precise pores), and sintering (particle fusion).<sup>55</sup>

Newer approaches and formats, using advanced manufacturing, include 3D printing, multi-layer melt extrusion, micro imprinting, and interfacial polymerization (thin-film composite layers), which achieve the desired morphology, pore size, and applications (e.g., filtration, gas separation).<sup>43</sup> It is a complex exercise on the SCPP relationship in polymer materials, incorporating processing parameters.<sup>56</sup>

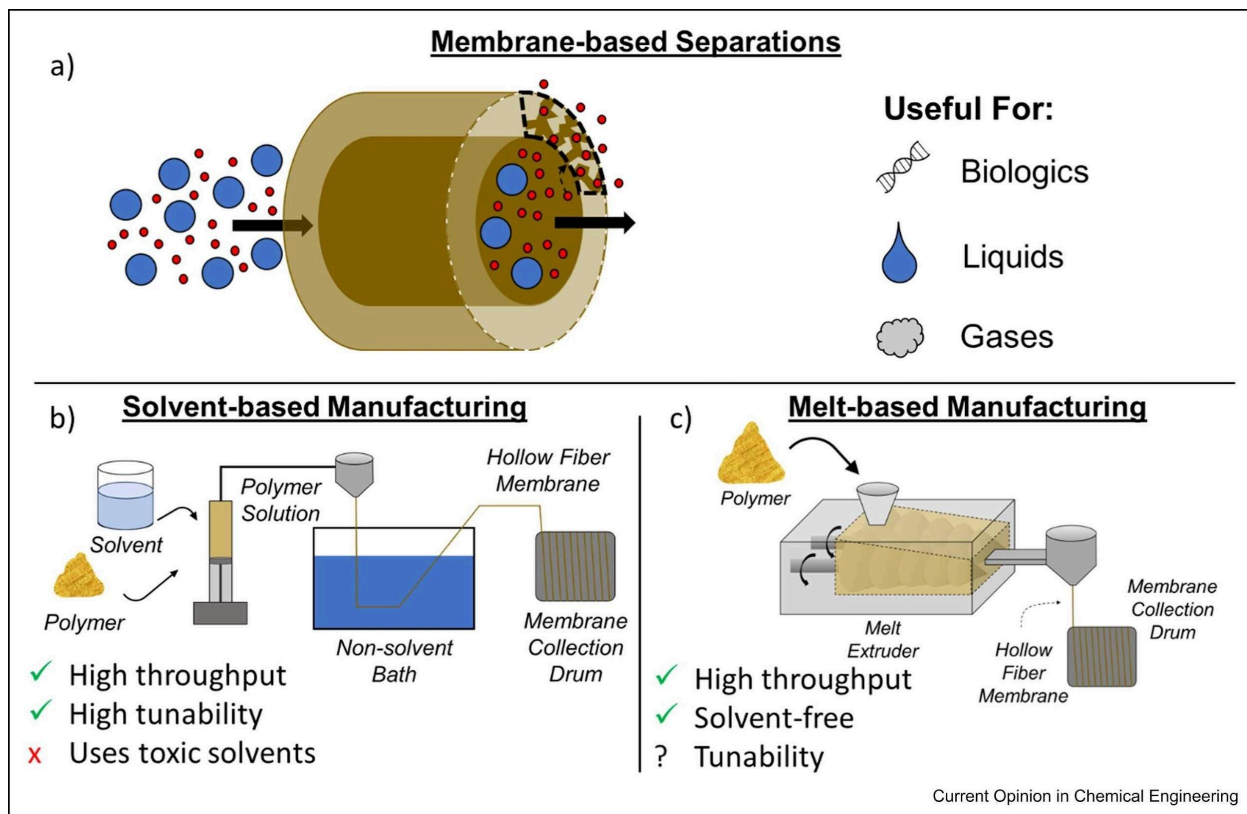


Figure 2. Summary of membrane manufacturing and testing. (a) Example of hollow fiber membrane operation. (b) Traditional solvent-based fiber spinning. (c) Melt extrusion + fiber spinning. (Figure and caption from reference<sup>57</sup> with no change under a Creative Commons 4.0 license<sup>58</sup>)

To summarize, the design and fabrication methods include the following.

- 1) Molecular and macromolecular design: classification as thermoplastic, thermoset, or elastomer. Also based on semi-crystalline or amorphous content, morphology, diffusion and transport behavior, and thermo-mechanical properties.
- 2) Solvent-based phase inversion (NIPS/VIPS): A polymer solution (dope) is cast, then immersed in a non-solvent bath (NIPS) or exposed to vapor (VIPS), causing phase separation and pore formation as solvent/non-solvent exchange.
- 3) Melt <sup>57</sup> and Electro-spinning: A melt polymer based on extrusion, quenching, or drawing, or a high voltage draws polymer solution into ultrafine fibers, creating nonwoven mats ideal for filtration and biomedical uses.
- 4) Stretching/Drawing: A solid polymer film (often phase-inversion-made) is stretched (cold or hot), inducing pores and increasing permeability.
- 5) Track Etching: Bombarding a polymer film with energetic ions creates cylindrical channels, which are then etched to form highly uniform pores.
- 6) Sintering: Heating powdered polymers (like PTFE, PE) below their melting point to fuse particles and form porous structures, common for chemically resistant membranes.
- 7) Interfacial Polymerization: A thin selective layer forms at the interface of two immiscible liquids, often used for high-performance thin-film composite (TFC) membranes (e.g., reverse osmosis).

Other related advanced techniques are as follows.<sup>56</sup>

- a). Advanced Melt Processing: Techniques such as melt-spinning, extrusion, and melt-pressing are used to process thermoplastic polymers, forming hollow fibers or flat sheets.
- b). Solution Casting/Evaporation: Casting polymer solutions and allowing solvents to evaporate, often used in labs, though less uniform than other methods.
- c). Template Synthesis (e.g., Block Copolymers): Using self-assembling block copolymers or colloidal templates to create highly ordered porous structures.
- d). 3D Printing and Lithography: Additive manufacturing and photolithographic techniques for complex, customized membrane geometries.
- e). Spray Coating: Depositing layers (like graphene oxide) from a spray, scalable but can lack uniformity.

Processing and fabrication implications may consist of the following factors.<sup>59</sup>

- 1). Morphology Control: Methods influence pore size, pore shape (finger-like, sponge-like), and skin layer thickness, affecting performance.
- 2). Additives: Chemicals like PVP or nanofillers are added to polymer solutions to control pore formation, increase hydrophilicity, and enhance properties.
- 3). Formats: Membranes are produced as flat sheets, hollow fibers, or spiral-wound modules.

## 4. Methods of Testing and Characterization.

Characterization of the polymer materials, characterization of processed or fabricated parts, and membrane performance testing are prerequisites, which may encompass characterization and validation for standardized performance, long-term, or environmental stability. Advanced characterization methods have emerged not only for membrane performance but also for *in situ* and real-time studies of their separation mechanisms.<sup>60</sup> They are sensitive to hierarchy in scale (molecular, mesoscopic, microscopic, and macroscopic) and can be varied with spatio-temporal considerations to match the observation objectives:<sup>61</sup> optical microscopy, probe microscopy (SPM, AFM), electron microscopy (SEM, TEM) for morphology, spectroscopy (FTIR, Raman, NMR, XPS) for chemical composition, and performance tests like flux/rejection measurements, pressure drop methods, permeability, and bubble-point/ thermoporometry for pore size, alongside XRD for crystal structure and mechanical tests (tensile) to assess surface/bulk structure, porosity, and separation efficiency for applications in water treatment, gas separation, etc.<sup>62</sup> Table 2 listed various common membrane characterization techniques.

Table 2. Membrane Characterization Techniques<sup>3,60-62</sup>

Category	Technique	Primary Function / Data Provided
Morphology & Structure	SEM	Visualizes surface topography, pore structure, and cross-sectional morphology.
	TEM	Provides high-resolution imaging of internal nanometer-scale features.
	AFM	Maps 3D surface topography and quantifies surface roughness.
	XRD	Identifies crystal structure, phase identification, and degree of crystallinity.
	SAXS/WAXS	Analyzes pore size distribution, particle size, and long-range structural order.
	Neutron Scattering	Probes structures using deuterated media to enhance contrast.

Chemical Composition	FTIR & Raman	Identifies chemical bonds, functional groups, and molecular vibrations.
	XPS	Determines surface elemental composition and chemical oxidation states.
	EDS / EDX	Provides elemental mapping and semi-quantitative analysis (via SEM).
	NMR	Probes molecular structure, chemical environment, and chain dynamics.
Porosity & Pore Size	Bubble-Point Test	Measures maximum pore size and distribution under wet conditions.
	Thermoporometry	Uses phase transitions of liquids in pores to calculate size distribution.
	MWCO	Defines the molecular weight at which 90% of a solute is rejected.
Performance & Transport	Filtration Tests	Quantifies water flux, solute rejection, and mass transfer permeability.
	Contact Angle	Measures surface energy to assess hydrophilicity and wettability.
	EIS	Evaluates ion transport, charge transfer, and membrane resistance.
Mechanical Properties	Tensile Testing	Measures ultimate strength, Young's modulus, and elongation at break.
	DMA	Analyzes viscoelastic behavior across temperature and frequency ranges.

## 5. APPLICATIONS

One application of membranes we highlight is membrane-based organic solvent separations, which will enhance the energy efficiency of existing separation and purification systems from crude oil to organic solvent waste.<sup>15,63,64</sup> Fractionating complex mixtures of organic molecules, such as crude oil, will reduce dependence on energy-intensive distillation or cracking ML algorithms and mass transport simulations can be integrated to predictively separate complex oil mixtures.<sup>37,65,66</sup> The use of ML predictors for molecular diffusion with transport simulation enables rapid screening of the best candidate polymer membranes for organic-organic separations.<sup>63</sup> Recent progress has been reported on the use of solution-processable polytriazoles. Efficient membrane-based hydrocarbon separations have been reported.<sup>66,67</sup> Progress has also been reported on the use of ultrathin polyamide films for controlled separations. These materials provide rapid transport for crude oil separation.<sup>68</sup> Table 3 provides additional information on membrane applications.

Table 3. Membrane applications by type and materials <sup>16,65,69–74</sup>

Category	Membrane Types & Materials	Key Function/Process
1. Water Filtration	MF/UF (PVDF, PES, Ceramic)	Removal of suspended solids and pathogens.
2. Municipal & Industrial High-Purity	RO/NF (Polyamide TFC, Polysulfone)	Brackish/wastewater treatment and softening.
3. Semiconductor & Pharma Water	RO/UF (Cellulose Acetate, Degas membranes)	Pyrogen-free water and ultrapure water (UPW).
4. Critical Minerals Separation	Supported Liquid Membranes (SLM), Ion-Exchange	Lithium/Cobalt recovery from brine or batteries.
5. Isotope Purification	Zeolite, Graphene, Polymer (Diffusion-based)	Separation of H <sub>2</sub> /D <sub>2</sub> and other isotopes.
6. Oil-Water & Emulsions	Ceramic, Janus (Hydrophilic/Oleophobic)	Breaking stable emulsions in oily wastewater.
7. Desalination	RO (Polyamide TFC), Membrane Distillation	Sea and brackish water conversion to freshwater.
8. Gas Separation & CO <sub>2</sub>	Polyimide, PIMs, Zeolites	Post-combustion carbon capture; N <sub>2</sub> /CH <sub>4</sub> separation.
9. Pervaporation	PVA, PDMS, Chitosan	Dehydration of alcohols and solvent recovery.
10. Organic Mixture Nanofiltration	Solvent Resistant NF (SRNF) (Polyimide, PBI)	Complex organic mixture/oil fractionation.

## 5.1 Functional Membranes, Coatings, and Nanostructured Composites

There has always been interest in introducing new materials, nanocomposites, functionality, and concepts for membrane transport and separation.<sup>42,56</sup> Important contributions from our group over the years include nanocomposite coating methods; non-wetting, anti-fouling, and de-icing capabilities for membranes and filters; efficient oil-water separators; and anti-corrosion coatings. We have reported on several papers that use the Cassie-Baxter phenomenon and approach<sup>75</sup> to enable superhydrophobicity and superoleophilicity in surface coatings, filters, and membranes. This is generally achieved by enabling surface heterogeneity, using nanocomposites, combining nanopatterning with electrodeposition of conducting polymers, and grafting polymers. Graphene oxide is the most important nanofiller, enabling membranes and coatings to exhibit outstanding properties.<sup>76</sup> New polymer and polyelectrolyte multilayer and layer-by-layer methods are important for demonstrating controlled diffusion, release, and even sensing with nanostructuring. The examples and discussions are provided as follows.

An important high-temperature thermoset is polybenzoxazine (PBZ), particularly for oil and gas applications.<sup>77</sup> Polybenzoxazine has exhibited excellent membrane and proton exchange membrane properties in electrolysis.<sup>78,79</sup> They have been employed for organic solvent microfiltration.<sup>80</sup> We first demonstrated the incorporation of silica nanoparticles with rubber-modified PBZ to fabricate superhydrophobic, superoleophilic coatings and filters via dipping or spraying, in which the coatings showed anticorrosion, anti-ice, self-cleaning, anti-bacteria, as well as organic-water separation properties.<sup>81</sup> Anti-corrosion properties on carbon steel were established from coatings fabricated from rubber-modified PBZ-based polyaniline composites.<sup>82</sup> Copolymers of epoxy and trifunctional PBZ also exhibit toughened thermo-mechanical properties.<sup>83</sup> A report on rubber-enhanced polymer materials highlighted the addition of elastomeric materials to boost the thermo-mechanical resilience of thermoset materials, such as polybenzoxazines.<sup>84</sup>

## 5.2 Vinyl polymers

Acrylate and methacrylate compositions that can be cross-linked by light or heat are desirable coating systems for membranes and filters since they are readily accessible and can be combined with nanoparticles to form robust nanocomposite films. For instance, a spray-coating technique was used with inorganic silica nanoparticles and photopolymerizable organic thiol-ene compounds to coat wire-mesh filters for oil/water separation.<sup>85</sup> The superhydrophobic coatings are self-cleaning and display excellent chemical resistance to various temperatures and pH conditions. In a previous work, fluorine-free superhydrophobic substances made with methacrylate monomers that include iso-norbornyl groups attained over 99% efficiency in extracting water from various oils and brines.<sup>86</sup> In another strategy, a fluorine-free superhydrophobic/ superoleophilic surface was developed via a two-step procedure involving dip-coating and oven curing of silica nanoparticles along with methacrylate monomers, for

which thermo-gravimetric analysis (TGA) techniques were employed to track reaction kinetics and superior wire-mesh adhesion was accomplished with different oils.<sup>87</sup>

### 5.3 Electrodeposition and Conducting Polymers

Electrodeposition is an efficient method for coating metal substrates. Electrically conducting and conjugated polymers, such as polythiophenes, polyaniline, and polycarbazoles are excellent anticorrosion materials as well.<sup>88,89</sup> Superhydrophobicity enables them to exhibit anti-fouling and non-wetting properties. At the same time, superoleophilicity allows them to be superior oil or wicking absorbers. We have demonstrated a number of electrodeposition and electropolymerization methods for depositing conjugated polymer films on metal and electrode surfaces, including wire-mesh filters.<sup>90-92</sup>

Robust oil-water separation was demonstrated using a one-step electropolymerized polythiophene coating, with which the resultant superhydrophobic and superoleophilic surface effectively separated six oil types across a wide pH range (1–14) and in brine.<sup>93</sup> Deposition on colloiddally nanopatterned surfaces resulted in superhydrophobic-superoleophilic with tunable wetting and electrochromic behavior.<sup>94</sup> We have reported on superhydrophobic-superoleophilic coatings from electropolymerized polythiophenes and polymer-grafted colloiddally nanopatterned surfaces,<sup>95</sup> which also exhibited hemi-wicking properties. In addition, the adaptability of patterned polymer brushes through electrodeposited atom-transfer radical polymerization (ATRP), reversible addition chain transfer (RAFT), and ring-opening metathesis polymerization (ROMP) on colloiddal template arrays was established.<sup>96</sup> An interesting study reported on the formation of free-standing, colloiddally nanopatterned Janus membranes based on conducting polymer–virus nanoparticle arrays.<sup>97</sup> Methods for electrochemically grafting polymer brushes onto electrode and metal surfaces were demonstrated and patented, achieving both anti-fouling and anti-corrosion properties in robust coatings for advanced membrane applications.<sup>98</sup>

### 5.4 Graphene and other Nanomaterials and Nanocomposites

Graphene, graphene oxide (GO), and reduced graphene oxide (rGO) are important classes of nanomaterials that exhibit electrical conductivity, barrier properties, and antimicrobial properties.<sup>99</sup> GO and rGO can be further functionalized through their hydroxyl and epoxide groups to expand their chemistry and utility in formulations and nanocomposites. They can be prepared as Janus nanosheets to exhibit bifacially distinct physico-chemical properties.<sup>100</sup> These can be used as nanofillers, additives, and functional groups for high-performance membranes and coatings. We have reported on the enhanced corrosion resistance and oil-water filtration characteristics of elastomer-modified polybenzoxazine/GO nanocomposite coatings.<sup>101</sup>

GO, and rGO nanoplatelets with nonpolar aliphatic groups of bifunctionalized displayed high corrosion resistance.<sup>102-104</sup> An efficient anti-corrosive coating was reported for epoxy resins with aromatic-functionalized rGO nanocomposites, thanks to the confinement of corrosive-ion transport.<sup>105</sup>

Furthermore, GO nanomaterials can undergo photoreduction, allowing the synthesis of graphene–metal nanoparticles, which can be important for hybrid membrane catalysis.<sup>106</sup> The

nanostructuring of GO and montmorillonite clay exhibited hydrogel and eventually aerogel properties for superior oil–water separation and oil cleanup.<sup>107</sup> Nanoclays are also of great interest for nanocomposite membranes and filters, as they exhibit anti-fouling and antibacterial behaviors.<sup>108</sup> We have reported the intercalation of polymerization initiators into these nanoparticles to enable free-radical vs. anionic *in situ* polymerization to build nanocomposites.<sup>109</sup>

GO nanomaterials and thiol-ene coatings offer excellent corrosion resistance and superhydrophobic, non-wetting properties.<sup>110</sup> Antimicrobial properties of a graphene-carbazole polymer (PVK-GO) nanocomposite film have been previously reported.<sup>111</sup> GO functionalized with ethylenediamine triacetic acid or EDTA presented excellent properties for heavy metal adsorption and anti-microbial function in a membrane.<sup>112</sup> In general, GO-nanocomposite materials can be used as filters to eliminate bacteria and heavy metals simultaneously, acting as chelators.<sup>113</sup> Chitosan-cross-linked GO coatings display an antimicrobial activity and could find applications in packaging.<sup>114</sup> Functionalized GO nanomaterials can be employed in a variety of compositions (with or without photoresins) and can be 3D printed for advanced membrane manufacturing.<sup>115</sup>

Nylons are important membranes for applications such as dialysis that require anti-fouling properties.<sup>116,117</sup> The combination of GO with nylons as membranes for molecular separations have been previously reported.<sup>118</sup> We have used selective laser sintering (SLS) together with a graphene-polyamide powder to fabricate metal-free plastic electric motors, and this is an crucial advancement for manufacturing metal-free parts with EMI conducting and shielding properties that can also be reverted to membrane fabrication.<sup>119</sup> SLS 3D printing was also used to fabricate a polyamide-12-carbon black composite that exhibited combined thermal and electrical conductivity in 3D printed parts.<sup>120</sup>

CNT nanomaterials are excellent for nanocomposites and coatings that confer antibacterial, nonfouling, and anticorrosion properties.<sup>121</sup> We demonstrated antimicrobial polycarbazole/CNT nanocomposite-coated membranes for water purification, and these membranes exhibit high filtration efficiency and bacterial toxicity, offering a significant advancement for filter design.<sup>122</sup> Patents based on polymer precursors for cross-linking with GO and CNT as films and coatings have been issued.<sup>123</sup>

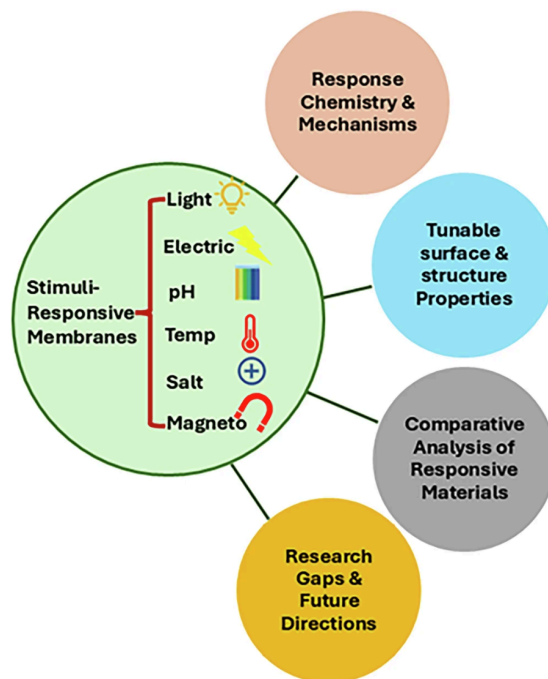
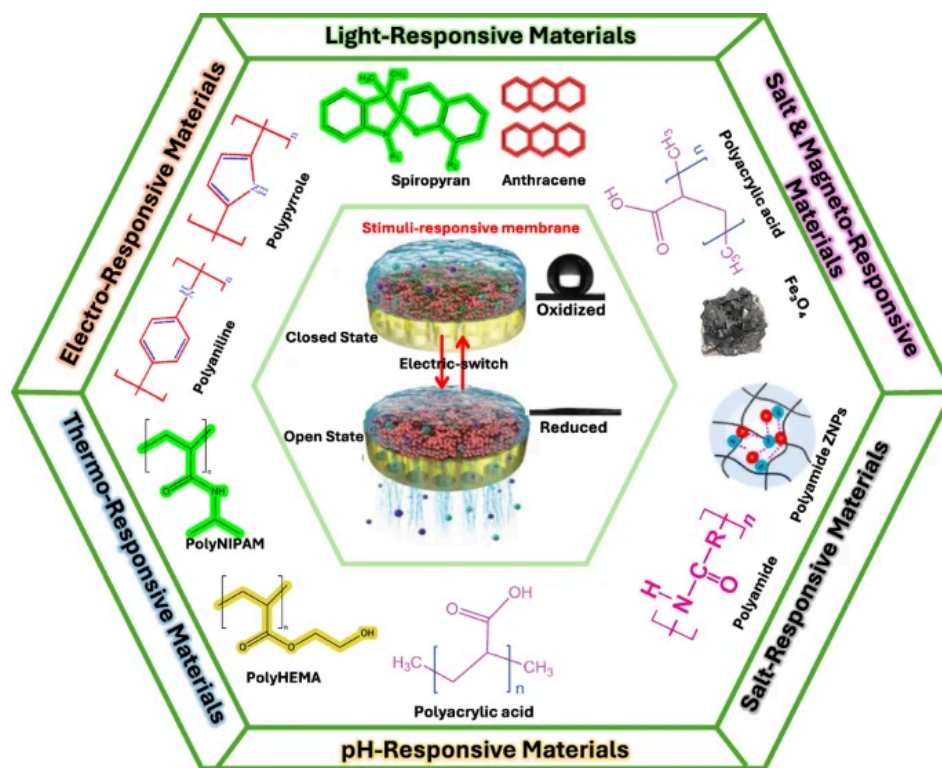


Figure 3. Classification and aspects of stimuli-responsive membranes (Figure from reference<sup>124</sup> with no change under a CC BY-NC-ND 4.0 license<sup>125</sup>)

## 5.5 Stimuli Responsive Systems

Stimuli-responsive polymers, smart coatings, and smart membranes enable multifunctionality even with high-performance applications or extreme environments (Figure 3).<sup>126</sup> In a recent review, smart, stimuli-responsive membranes have shown potential for electro-, pH-, temperature-, and other field-gradient stimuli, enabling resilient multifunctionality.<sup>124</sup> This can resonate well with applications in the oil and gas industry, which are needed in challenging environments.<sup>127</sup>

Stimuli-responsive properties can be observed in coatings (which we have widely reported with controlled wetting) and in particles and polymers with thermal and shape-memory properties.<sup>128,129</sup> In 3D printing, the combination with stimuli-responsive materials is also called 4D printing. We have reported on mechanically robust, ultra-hierarchical 3D-printed foams that exhibit ultra-elastic deformation over 1000 cycles and tunable rigidity, both determined by composition and open-cell porous structure.<sup>130</sup> 4D Printing was carried out on a polybenzoxazole-epoxy composition containing CNT, which exhibited shape-memory characteristics with high cyclic recovery.<sup>131</sup>

## 5.6 Polyelectrolytes and Multilayer Complexes

Polyelectrolytes and polyzwitterions are important membrane materials because they can mediate ion-transport.<sup>132</sup> Polyelectrolyte complex membranes can be prepared as coacervate or polyelectrolyte multilayers (PEM).<sup>133</sup> They can exhibit anti-fouling control, stimuli-responsiveness, ion selectivity, and high permeance; they have been used as proton-exchange membranes for fuel cells, ion-exchange membranes for flow batteries, RO membranes, and for wastewater filtration.<sup>7,17,133</sup> A PEM or multilayer complex of oppositely charged polyelectrolytes is a promising thin-film membrane.<sup>134</sup> We have investigated the properties of polyelectrolytes and multilayer films, including combinations with other self-assembly and polymer- synthesis methods, to elucidate their behavior. The following are examples:

We have investigated polyzwitterion hygroscopic films in electric fields using neutron and X-ray reflectometry.<sup>135</sup> It is essential to probe the nature of chemical specificity in polyzwitterion-polyelectrolyte complexes, where pairing with either polycations or polyanions results in a stronger charge interaction.<sup>136</sup> An anti-polyelectrolyte and polyelectrolyte behavior was identified, which influenced the conformation of polyzwitterionic chains in dilute aqueous solutions as confirmed by X-ray scattering.<sup>137</sup> One possible application of polyelectrolyte materials is in Li-metal battery applications: for example, a high-entropy gel-polymer electrolyte was reported, with a high-temperature operational range and excellent cyclic stability.<sup>138</sup>

Most of our work on polyelectrolyte complexes has focused on demonstrating the unique properties of ultrathin film PECs prepared by layer-by-layer (LBL) deposition and as core-shell particles, which can exhibit distinctive ion-diffusion, electron transport, optical, and gas-sensing properties.<sup>139</sup> These ultrathin films have great versatility in composition and fabrication for PEM membrane applications.<sup>133</sup> Among the properties we emphasized was ion transport, including pH-sensitive bipolar ion permeability.<sup>140</sup> The ability to induce photo-alignment or photoisomerization in polyionic azobenzene-containing LBL thin films was reported

previously.<sup>141</sup> We also reported on the electrical and gas-sensing characteristics of copper phthalocyanine LBL films.<sup>142</sup> An electrostatic LBL method was used to construct fibrous TMV biofilms.<sup>143</sup>

Combining LBL films with surface-initiated polymerization (SIP) allowed us to control grafted polymer density and functionality, and we applied this technique to fabricate stimuli-responsive binary mixed brushes and free-standing films.<sup>144</sup>

Films of semifluorinated block copolymer brushes derived from LBL-PEM macroinitiators demonstrated controlled wetting behavior within each block and at different grafting densities.<sup>145</sup> They can also be prepared as free-standing membrane films. We reported on stimuli-responsive polymer films with a binary architecture which display switchable pH and temperature responsiveness.<sup>146</sup> Using the LBL method and ATRP grafting of polyNIPAM brushes, we showed a reversible superhydrophilic and superhydrophobic activity on a bioinspired lotus-leaf pattern.<sup>147</sup>

Colloidal particles enable the LBL method to produce unique transport and guest-host particle systems with complex polyelectrolyte shells.<sup>148</sup> Applications of these core-shell and hollow shell particles have been widely reported.<sup>149,150</sup> The fascinating concept of core-shell particles and their respective applications as colloidosome microcapsules has been reported.<sup>151</sup> Their analogy as biological templates and prospective applications for drug delivery and membranes has been suggested.<sup>152</sup>

Our contributions in these areas were in developing chemistries and materials for controlled transport and synthesis. In a previous study, we report on the sustained release control of small molecules by means of benzophenone photo-crosslinking on polyelectrolyte LBL hollow capsules.<sup>153</sup> The LBL-PEM assembly of polyaniline and sulfonated polystyrene as multilayered core-shell and hollow-shell colloidal particles displayed promising redox ion transport control.<sup>154</sup> Using a photo-crosslinking procedure, we generated luminescent spherical and hollow-shell particles for controlled drug delivery, while combining LBL-PEM and SIP-ATRP on these particles created a ternary system with dual stimuli-responsive shells.<sup>155</sup>

Conducting polymers (polypyrrole, polyaniline, polythiophene, and others) have ion-transport membrane applications.<sup>156,157</sup> Proton conductivity has been reported for composite polyelectrolyte-MOF membranes in fuel cell applications.<sup>158</sup> The intriguing concept of using REDOX control transport in LBL-PEM and conducting polymer films indicates fine ion-transport control through doping of conducting polymers. We pioneered methods for preparing electropolymerizable LBL-PEM films with electropolymerizable side groups from polyelectrolyte via cyclic voltammetry or potentiostat methods.<sup>159</sup> The electrochemical cross-linking of LBL-PEM-carbazole precursor films was established using conducting atomic force microscopy (C-AFM).<sup>160</sup> They also exhibited patterning properties via lithographic or non-lithographic methods.

## 5.7 Multilayer Extruded Films

Multi-layered extruded polymer films are an important technology that was developed to show a co-extrusion of incompatible but melt-indexed polymers.<sup>161</sup> They can have a variety of

morphologies, compositions, anisotropic orientations, in addition to the ability to form open cell structures.<sup>162,163</sup> More importantly, these films exhibited excellent gas-separation membrane properties, including high CO<sub>2</sub>/O<sub>2</sub> selectivity and gas flux, with two distinct polymer layers playing a key role in combining these properties.<sup>164</sup> When subjected to biaxial stretching, they also exhibited excellent membrane and separation properties.<sup>165</sup> We have demonstrated swellability and controlled characteristics in these films by employing guest-host system principles, as well as the capability to create various particle shapes using reactive ion etching.<sup>166,167</sup>

Electrospinning of polystyrene (PS) and CNT nanofibers has resulted in superhydrophobic and antibacterial behavior in these multilayer films, which can also serve as gas barrier films.<sup>168</sup> We also demonstrated stimuli-responsive polymer characteristics with grafted poly(N-isopropylacrylamide) (PNIPAM) brush layers on coextruded, nanolayered polystyrene (PS)/polycaprolactone (PCL) films.<sup>169</sup> Innovative characterization for polymer coatings and polymer-dielectric (solvent) interactions, including sum-frequency generation (SFG), is possible in conjunction with solvent swelling and interaction on surfaces.<sup>170</sup>

## 6. Introduction to AI/ML

### AI and the machine learning ecosystem

Artificial Intelligence (AI) is the overarching discipline of creating computational systems that exhibit behavior traditionally associated with biological intelligence.<sup>29,171,172</sup> This includes everything from the symbolic logic of early "expert systems" to the probabilistic models used today. Machine Learning (ML) is the most successful branch of AI, characterized by a shift from hand-coded rules to statistical inference. In ML, models learn from data by minimizing a loss function—essentially a mathematical "penalty" for incorrect predictions. Data science provides the experimental framework for this, managing the data-cleaning, feature engineering, and rigorous statistical validation pipelines required to make these models reliable.

Machine learning is traditionally categorized by the nature of the feedback the model receives during training.<sup>29,171,172</sup> (1) Supervised Learning: The model is "taught" using labeled datasets. Algorithms like decision trees split data into branches based on feature values, while support vector machines (SVMs) find the optimal boundary (hyperplane) to separate classes. (2) Unsupervised Learning: The model identifies patterns without labels. Clustering (e.g., K-Means) groups similar data points, while dimensionality reduction techniques like principal component analysis (PCA) simplify complex datasets by identifying the most influential variables. (3) Reinforcement Learning (RL): Inspired by behavioral psychology, an agent learns to make

sequences of decisions by receiving rewards or penalties. This is the foundation for robotics and game-playing AI.

Natural Language Processing (NLP) has been revolutionized by the shift from recurrent architectures to the Transformer architecture.<sup>23,24,173–175</sup> Transformers use a protocol called "Self-Attention" to process entire sequences of text simultaneously, understanding how every word relates to every other word regardless of distance. LLMs are massive neural networks trained on trillions of tokens. They function as high-dimensional probability engines; when you ask a question, the model isn't "thinking" in the human sense but rather calculating the most statistically probable sequence of characters to follow your prompt. Beyond text, these architectures are being applied to "biological languages," such as SMILES strings in chemistry, allowing AI to "write" new molecular structures for drug discovery.

The most recent paradigm shift is the move toward Agentic AI.<sup>30,176–179</sup> While a standard LLM is a passive tool (it waits for a prompt and provides a static response), an AI Agent is an autonomous system that uses an LLM as its "brain" to interact with the world. An agentic system typically consists of four core components: (1) Reasoning/Planning: The LLM breaks a complex goal (e.g., "Research and buy the best laptop for my budget") into a series of logical sub-tasks. (2) Memory: Short-term memory (in-context learning) and long-term memory (vector databases/RAG) allow the agent to learn from its mistakes and retain information across long workflows. (3) Tool Use: The agent is granted "hands"—the ability to call APIs, search the web, execute Python code, or access local files. (4) Action/Refinement Loops: The agent observes the outcome of its actions and loops back to correct its plan if the result wasn't as expected.

## **AI in the context of other simulations**

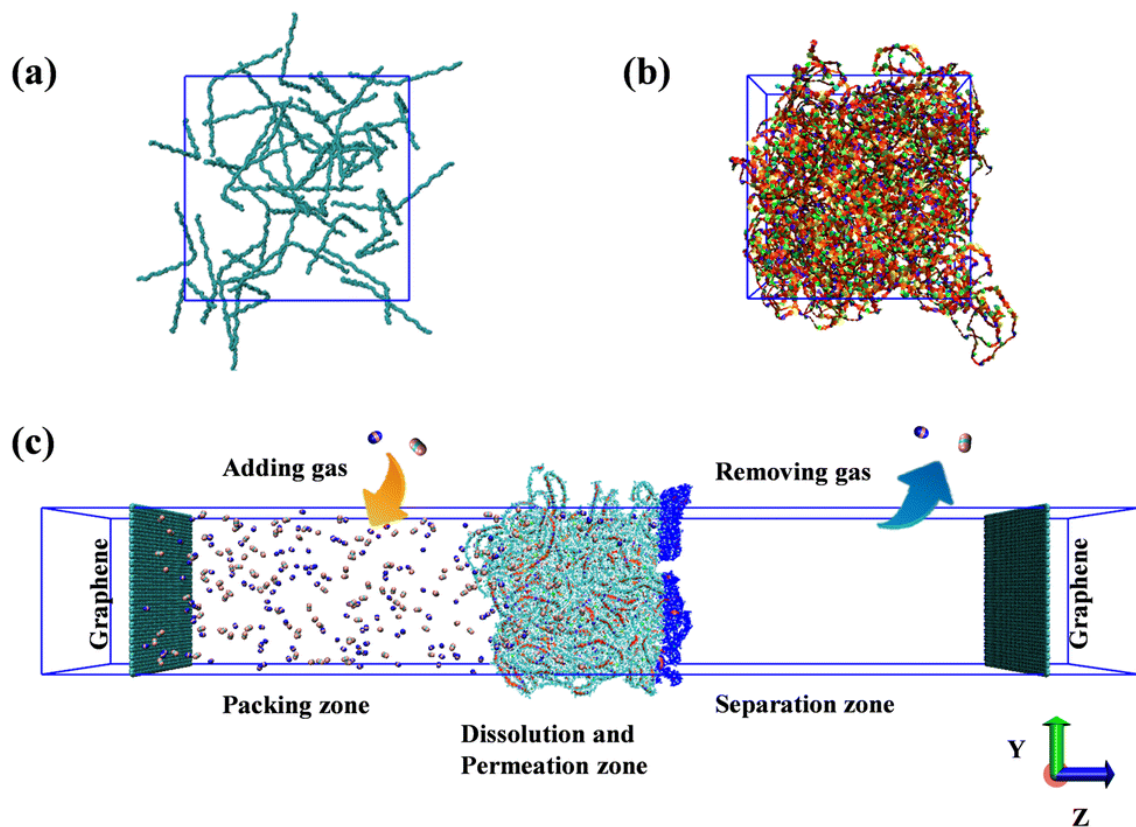
The exploration of new materials leverages ML-driven simulation to reduce computational costs and optimizes feedback using reinforcement learning.<sup>28,30,33,171,172</sup> Digital twins provide end-to-end AI/ML simulation workflows for these stages, enabling inverse design across material properties, membrane fabrication, process engineering, and performance. Membrane simulation methods span multiple scales, from atomistic density functional theory (DFT) and quantum mechanics to molecular dynamics (MD) for detailed field interactions. Larger systems utilize faster coarse-grained (CG) MD, while Dissipative Particle Dynamics (DPD) and Monte Carlo (MC) methods address mesoscale structures and statistical sampling, respectively—often integrated with high-level Computational Fluid Dynamics (CFD). Furthermore, AI/machine learning enables multiscale modeling of complex processes such as water purification, transport, and fouling. An extended classification of membrane simulations is given as follows.

### **A. Molecular-level methods:**

1. Molecular dynamics (MD): Simulates atomic motions over time, using all-atom (AA) or coarse-grained (CG) models to study protein-lipid interactions, membrane dynamics, and transport mechanisms.
2. Ab Initio/DFT: For quantum-level interactions, often used for specific site studies.

3. Dissipative Particle Dynamics (DPD): A coarse-grained particle-based method capturing hydrodynamic interactions, ideal for large-scale mesoscale phenomena like membrane formation.

4. Monte Carlo (MC): A statistical method for exploring system configurations and properties, often combined with MD. An example was given in a previous work on a PIM membrane where the gas separation mechanism was established in the context of microporosity, adsorptive characteristics, selectivity, and diffusive transport.<sup>180</sup> (Figure 4)



**Figure 4** (a) The initial low-density simulation box; (b) the simulation box after 21-step MD compression; (c) the gas diffusion model of membranes with a constant concentration gradient. (Figure and caption from reference<sup>180</sup> with no change under a Creative Commons BY-NC 3.0 license<sup>10</sup>)

B. Mesoscale and Coarse-Grained Methods:<sup>181,182</sup>

1. Coarse-Grained MD (CGMD): Groups atoms into "beads" to simulate larger systems faster, improving efficiency while maintaining chemical detail at interfaces.
2. Highly Mobile Membrane Mimetic (HMMM): An accelerated MD approach replacing some lipid tails with solvent for faster lipid diffusion.

C. System-Level & Multiscale Methods:<sup>64</sup>

1. Computational Fluid Dynamics (CFD): Models fluid flow, concentration polarization, and fouling at the continuum level, often coupled with molecular simulations.
2. Finite element analysis (FEA): Often used for a microscopic phenomenon and thermo-mechanical properties

D. Artificial Intelligence (AI) and Machine Learning (ML): Used with simulation data to predict intrinsic and extrinsic properties, accelerate design, use of new composites, and optimize performance.<sup>183</sup>

E. Process and Macroscopic Methods:<sup>184</sup>

1. Process Simulators: Models entire separation units, flow behavior, sometimes requiring custom equations for membrane units.
2. Finite Difference/Element Models and Response Surface Methodology (RSM): For system-wide performance and optimization.

These methods are often combined in multiscale frameworks to bridge scales, from atomic details to industrial process performance, enabling rational design of next-generation membranes. (Table 4) An end-to-end digital twin will be ideal (Figure 5).<sup>185</sup>

Table 4. Multiscale membrane simulation methods discussed in this section

Scale & Category	Technique	Primary Function / Key Application
Molecular Level (Quantum)	Ab Initio / DFT	Quantum-level studies of specific binding sites, adsorption energies, and electronic interactions.
Molecular Level (Atomistic)	All-Atom MD	Simulates exact atomic motions to study protein-lipid interactions and specific transport mechanisms.
	Monte Carlo (MC)	Statistical sampling of system configurations; vital for predicting gas adsorption and solubility.
Mesoscale & Coarse-Grained	CGMD (Coarse-Grained MD)	Groups atoms into "beads" to simulate larger systems (>100 nm) and longer timescales while retaining chemical detail.
	DPD (Dissipative Particle Dynamics)	Captures hydrodynamic interactions; ideal for modeling membrane formation and phase separation.
Continuum & System Level	CFD (Computational Fluid Dynamics)	Models fluid flow, concentration polarization, and fouling patterns at the membrane-fluid interface.
	FEA (Finite Element Analysis)	Evaluates thermo-mechanical properties and microscopic stress/strain phenomena.
	Process Simulators	Models entire industrial separation units; often requires custom equations for specific membrane modules.
Advanced Optimization	AI and Machine Learning	Predicts material properties and optimizes composite designs by analyzing large simulation or experimental datasets.
	RSM (Response Surface Methodology)	Statistical methods used for system-wide performance optimization and experimental design.

Data generated from surrogates or simulations—ranging from targeted datasets to ideal outcomes—can be tailored to specific applications. Furthermore, digital twins and Large Language Models (LLMs) can generate predicted outcomes to facilitate essential feature extraction from membrane data. By employing featurization or fingerprinting, membrane architectures and properties are encoded into numerical vectors, enabling their integration as input features for ML-based predictive modeling.<sup>186</sup> Membrane featurization strategies are tailored to specific materials—accounting for polymer types and their physicochemical properties—and dictate the selection of appropriate machine learning architectures. By utilizing regression methods, Bayesian optimization, or neural networks, ML models can efficiently narrow the search space to identify the most promising membrane candidates.<sup>187</sup> The SHAP package can be useful for quantitatively analyzing the correlation of membrane features and transport properties.<sup>188</sup> This approach enables the refinement of molecular architectures in conjunction with polymer chemistry and physical properties. For instance, it allows for the determination of key correlations between RO and NF membrane descriptors and critical performance metrics, such as ion rejection efficiency.

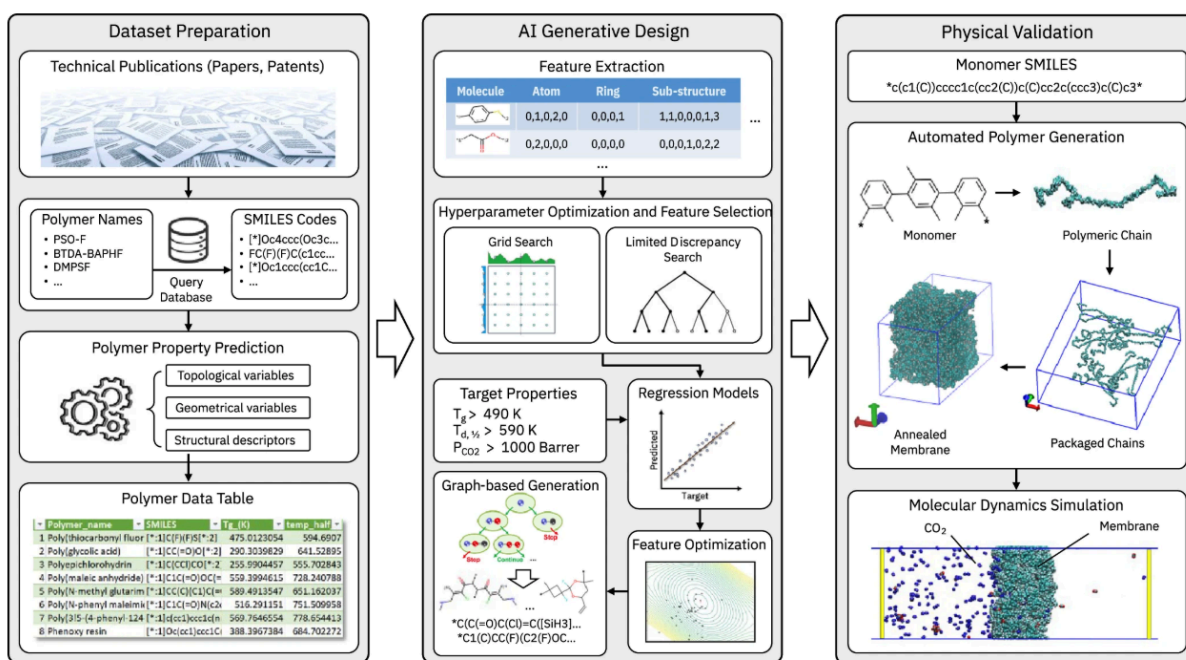


Figure 5. The workflow consists of training dataset preparation, ML-based generative monomer design, and physical validation of polymer based gas filtration with molecular dynamics simulations. (Figure and caption from reference<sup>185</sup> with no change under a Creative commons license 4.0<sup>58</sup>)

Computational strategies for nanofiltration and ultrafiltration leverage nanopore modeling, density functional theory (DFT) calculations, molecular dynamics (MD), and materials-based Large Language Models (LLMs). Within this framework, regression models are employed to predict critical thermodynamic parameters, such as the enthalpic ( $\Delta H^\ddagger$ ), entropic ( $T\Delta S^\ddagger$ ), and free-energy barrier ( $\Delta G^\ddagger$ ) parameters for ion permeation, for example. Other feature subsets can be chosen by applying a recursive feature addition and regression-based coefficients.<sup>189</sup> These features encompass critical parameters such as pore size, capillarity, surface energy, and hydrophilicity, all of which fundamentally dictate the permeability, ion transport kinetics, and selectivity of the membrane.<sup>190</sup> These AI/ML workflows enable the accurate prediction of critical performance metrics, including permeate flux, rejection rates, and fouling tendencies. Ultimately, such predictive capabilities facilitate a deeper understanding of membrane behavior and material properties tailored for specific industrial applications.

By leveraging machine learning models, researchers can now develop automated pipelines for high-throughput material selection and characterization. Specifically, the integration of Bayesian optimization, convolutional neural networks (CNNs), artificial neural networks (ANNs), and deep reinforcement learning (deep RL) has become instrumental in accelerating the discovery and optimization of nanoporous materials (Figure 5).<sup>191</sup>

Better ML models will be developed through simulation, and more empirical data of membranes and performance will be obtained; a data-driven science discovery phase will prevail.<sup>192</sup> There are both challenges and opportunities for this:

- 1) The lack of data sets will prevent the transition to more DL models and computer vision methods
- 2) Standardized data representation and model training can be made more available to computational chemists, resulting in better data sets. Consistency of labels, featurization, descriptors, experimental parameter prediction, and evaluation methods for membrane design will be helpful.
- 3) Modeling and ML of composite and nanocomposite formulation and behavior need to be addressed since they are becoming more important as a class of membranes.<sup>193</sup>
- 4) The development of multi-objective simulations is essential to ensure that computational models remain fit-for-purpose and aligned with specific membrane applications. For example, in gas separation, membranes can be selective to multiple gas types, requiring a multiobjective optimization approach. The same applies to wastewater treatment and filtration.<sup>194</sup>

Resolving these challenges will enhance the use of ML-assisted membrane simulation and design.<sup>195</sup> Moreover, automated laboratory techniques will enable acceleration of material discovery, including the use of nanomaterials and nanocomposites.<sup>196</sup> By designing a workflow that enables an LLM to autonomously plan, design, and execute complex experiments, future automated labs will promote significant advancements in the field, enabling new membrane applications in water purification, desalination, gas separation, biomedical devices, and pervaporation technologies (Figure 6).<sup>197,198</sup>

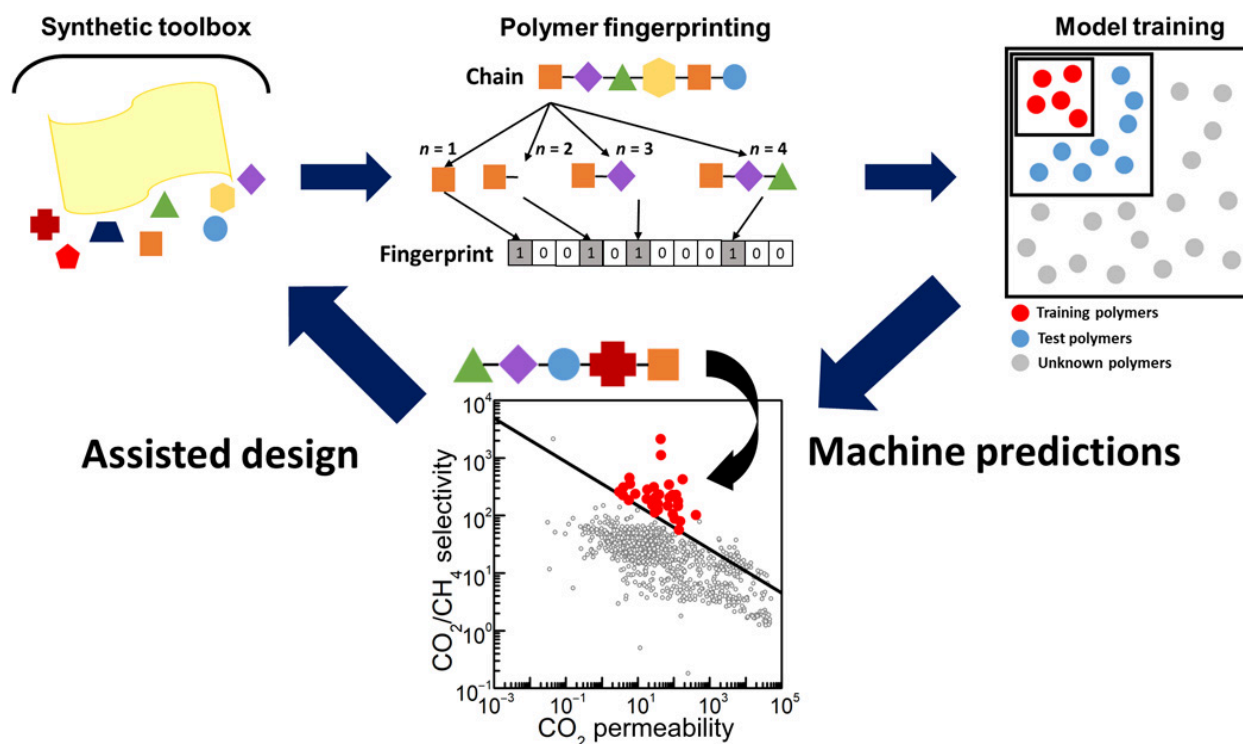


Figure 6. Assisted design of high-performance polymer membranes. The large synthetic toolbox available for creating new polymers is simulated by translating the polymer into a binary “fingerprint,” which is input to the ML algorithm. The model is trained with a random subgroup of polymers from our literature database and then tested against the remaining polymers. The model is then applied to a large set of literature data to discover high-performance polymers, thus facilitating machine-assisted design. (Figure and caption from reference<sup>199</sup> with no change under a creative commons license 4.0<sup>58</sup>)

## 7. 3D Printing and Membrane Research

3D printing, or additive manufacturing (AM), is classified primarily by how material is deposited and solidified.<sup>26,200–204</sup> For most industrial and consumer applications, the landscape is dominated by Vat Photopolymerization (using light-curable resins), Material Extrusion (melting filaments), and Powder Bed Fusion (fusing particles with lasers). Each classification is defined by its “energy source” (laser, heat, or chemical binder) and the physical state of the starting material. The materials used in these processes have expanded from simple plastics to high-performance composites, metals, and ceramics. Thermoplastics like PLA, ABS, and high-strength PEEK remain the workhorses for extrusion-based methods.<sup>202,205</sup> In contrast, photopolymer resins allow for incredible detail and smooth surfaces in dental and biomedical applications.<sup>206–208</sup>

There is high potential for additive manufacturing and 3D printing of membranes and filters.(Figure 7) Additive manufacturing enables the fabrication of complex membrane media and customized filter architectures, allowing for the development of material form factors precisely tailored to specific functional applications.<sup>209</sup> 3D printing, together with other forms of fabrication based on formative or subtractive manufacturing, can fully develop a new design concept for a membrane or filter. We have previously reviewed the opportunities of 3D printing for membrane separation, desalination, and water purification applications.<sup>200</sup> These manufacturing capabilities offer significant potential for the fabrication of novel filtration membranes, adsorbents, desalination components, and modular spacers. Furthermore, this approach facilitates the design and rapid prototyping of innovative filter media and geometries for applications in water purification, solar steam generation, and the development of porous catalyst supports.<sup>210</sup> The adaptation of advanced manufacturing methods, including 3D printing, is crucial to many other industries that also support environmental sustainability in a circular economy.<sup>201</sup>

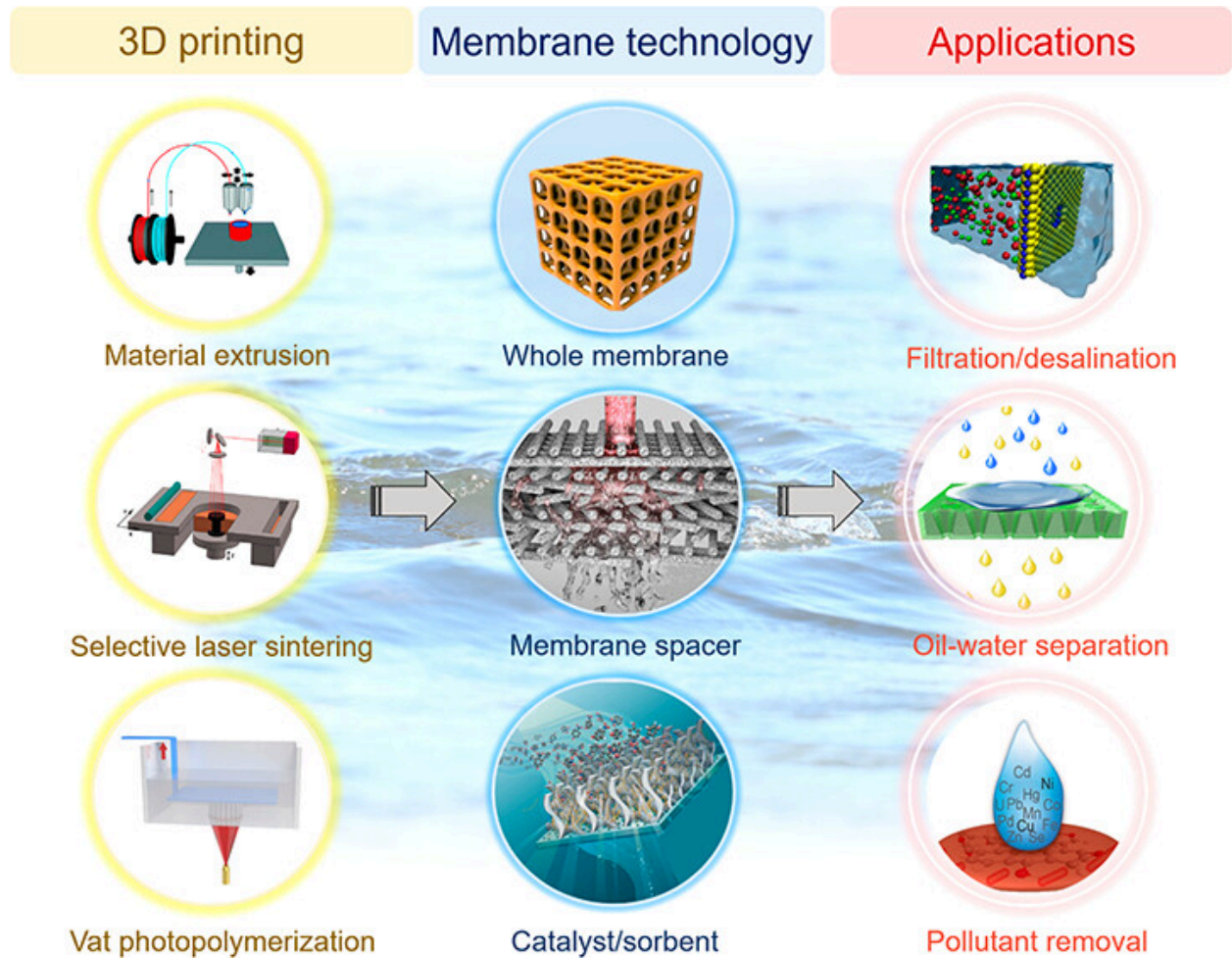


Figure 7. 3D printed membranes. (Figure from reference<sup>211</sup> with no change under a CC BY-NC-ND 4.0 license<sup>125</sup>)

Our previous work has detailed various 3D printing materials, methods, and applications, specifically focusing on thermoplastic polymers and nanocomposites. By highlighting the potential for creating toughened materials with diverse fabrication pathways, these investigations serve as a necessary foundation for understanding the material properties and processing capabilities vital for 3D-printed polymer systems.<sup>202</sup> There are many novel opportunities to employ thermoplastics, thermosets, and elastomers (silicone, polyurea, polyurethane<sup>212</sup>) in advanced manufacturing, as has been reported.<sup>130,213,214</sup> In particular, Direct Ink Writing (DIW) 3D printing relies on shear-thinning behavior and precisely tuned rheological properties to achieve high-resolution prints; the effectiveness of this approach was demonstrated by successfully printing commercial styrene-butadiene rubber (SBR) and moisture-curable polyurethane inks.<sup>215,216</sup>

Polypropylene (PP), an important membrane and thermoplastic material, has been optimized for 3D printing by annealing to optimize its thermomechanical properties.<sup>217</sup> Polyethylene terephthalate (PET) is also an excellent thermoplastic membrane and filtration material, together with polyethylene terephthalate glycol PETG.<sup>218,219</sup> We have demonstrated 3D printing and post-processing of PETG materials with superior thermo-mechanical properties.<sup>220</sup>

A review of additive manufacturing of viscoelastic materials, including hydrogels, and their flow behavior has been reported.<sup>221</sup> A number of these materials are also bio-based and are important for hydrogel and bio membrane applications.<sup>222,223</sup> Thermo-mechanical and swelling characteristics were investigated for 3D printed poly (ethylene glycol) diacrylate/silica nanocomposites.<sup>224</sup>

The 3D printing of high-performance polymeric (HPP) composites is important for the oil and gas industry, an industry that uses a lot of membrane technologies.<sup>225</sup> PEEK-based membranes give excellent thermo-mechanical and chemical stability they have been used for organic solvent separations, showing good permeance and rejection rates even at high temperatures.<sup>226</sup> We have reported on the 3D printing of PEEK by optimizing its thermal processing and mechanical properties.<sup>227</sup> Optimization can also be achieved by controlling slicing parameters and analyzing void content using X-ray microcomputed tomography.<sup>228,229</sup>

Another important HPP membrane material is polyphenylene sulfone (PPSU) and polysulfone (PSU), and some have reported applications in water-in-oil emulsion separations.<sup>230–232</sup> We have reported on their 3D printability by correlating viscosity and die-swell behavior in 3D-printed parts to optimize their thermo-mechanical properties.<sup>233</sup>

Silicone polymers are excellent gas membranes and separation materials.<sup>234–236</sup> They have been used for oil-water separations, membrane actuators, and as coatings for other membranes to provide chemical stability.<sup>237–239</sup> Specifically, for gas-separation membranes: CO<sub>2</sub>/N<sub>2</sub> separation, we highlighted the use of DIW 3D printing to fabricate formulated silicone/silica nanoparticle materials with the right form factor; it was observed that the PDMS-based membranes exhibited high CO<sub>2</sub> permeability with slightly lower selectivity for the CO<sub>2</sub>/N<sub>2</sub> separations.<sup>240–242</sup>

We first reported on the optimized 3D printability of commercial silicone-based adhesives with high resolution and thermo-mechanical stability.<sup>243</sup> Salt/silica PDMS formulations with controlled porosity were printed to create multifunctional, hyperelastic materials for oil-water separation and spill cleanup.<sup>214</sup> By systematically formulating silicone elastomeric inks, we demonstrated their commercial viability by correlating ink composition with key properties such as conductivity, viscosity, elasticity, and thermal stability.<sup>244</sup> To further optimize the formulation, carbon nanotubes (CNTs) were incorporated to precisely control gelling and curing behavior during the 3D printing process.<sup>245</sup> An additional method to 3D print silicones was to incorporate them into methacrylate photoresins using SLA printing at loadings up to 20%.<sup>246</sup> We recently reviewed advanced silicone materials and their application, including soft actuators.<sup>247</sup>

We highlight the critical role of statistical methods—such as simulation-based optimization, factorial design, and Taguchi methodology—in the systematic fabrication and characterization of 3D-printed polymers.<sup>248</sup> Building upon established methods such as injection molding,

thermoforming, and reaction injection molding, we demonstrate the utility of 3D-printed molds for rapid tooling and process adaptation.<sup>249,250</sup> It is also feasible to design micro-sandwiched structures via DIW to show multi-layer reinforcement in composites when combined with 3D printing.<sup>251</sup>

Nanocomposite membranes offer many new functionalities for separation and also provide strong thermomechanical reinforcement.<sup>252</sup> We have summarized advanced and functional nanocomposite materials and their importance in advanced manufacturing in a previous work.<sup>203</sup> An earlier review of 3D-printed polymer nanocomposites via stereolithographic (SLA) or digital light processing (DLP) was reported, focusing on future opportunities for materials research based on photopolymerizable resins.<sup>253</sup> Cellulose and other polysaccharide nanocrystals, carbon nanotubes (CNT), graphene nanomaterials, clay nanoparticles, and other nanoparticles were important additives for SLA 3D printing due to their ability to improve thermomechanical properties.<sup>254–257</sup> The 3D printing of methacrylate/chitin nanowhisker composites via SLA reveals that even low loadings (0.5 wt%) of chitin nanowhiskers substantially enhance the thermo-mechanical performance of the printed structures.<sup>258</sup> The DIW 3D printing of thermally cured rubber-toughened epoxy was made possible by polybutadiene addition (Figure 8), with shape memory properties.<sup>259</sup> The superior thermo-mechanical properties of epoxy/carbon fiber (CF) composites based on surface-functionalized CF were demonstrated.<sup>260</sup> Furthermore, CF-reinforced epoxy composites were 3D printed by incorporating helicoid channels for passive fiber alignment control, with FEA modeling.<sup>261</sup>

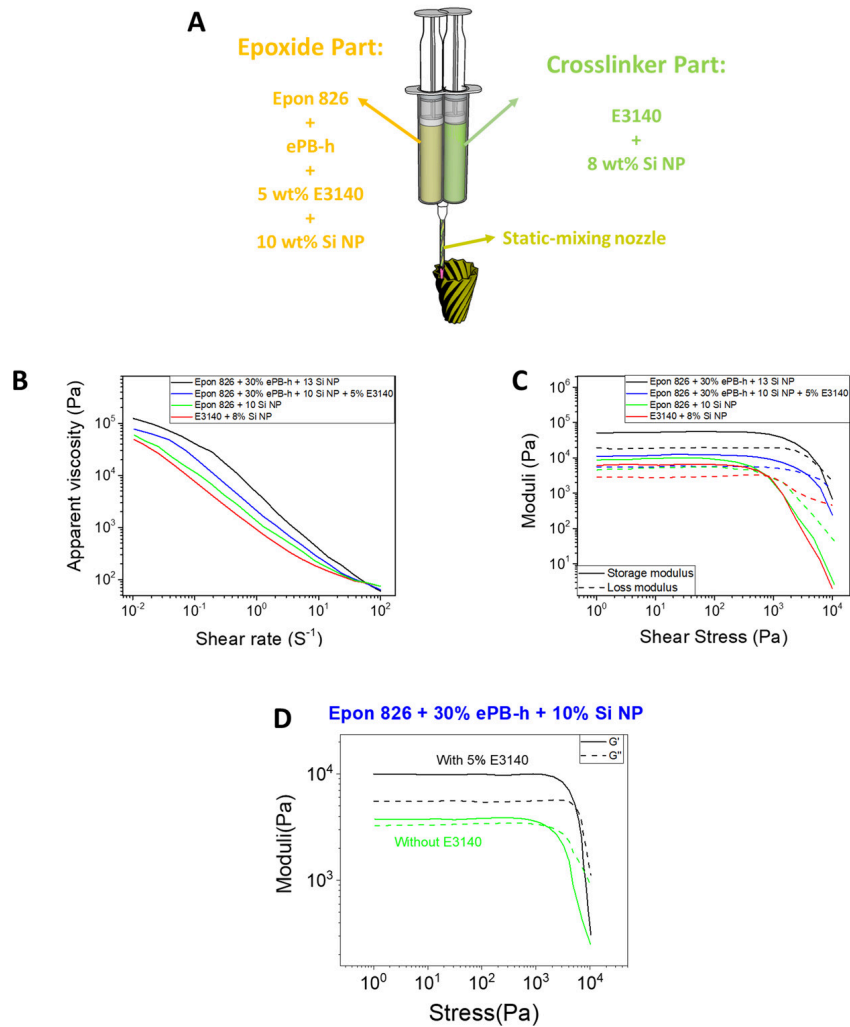
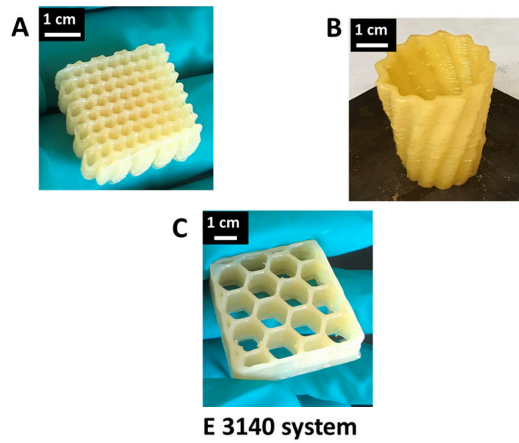


Figure 8. **Top:** Optical images of 3D printed epoxies. (A) Lattice structure printed from the E3140 system with 30 wt % ePB-h. (B) Vase printed from the W agent system with 20 wt % ePB-h. (C) Honeycomb structure printed from the E3140 system with no ePB-h. **Bottom:** (A)

Schematic illustration of the printing process of the E3140 system. (B) Viscosity of the epoxide and cross-linker parts with different loadings of silica NP. (C)  $G'$  and  $G''$  of the epoxide and cross-linker parts with different loadings of silica NP. (D)  $G'$  and  $G''$  of the epoxide resin part with and without 5 wt % E3140. (Figure and caption from reference<sup>259</sup> with no change under author reuse permission from ACS. Copyright © 2020 American Chemical Society)

The 3D printing of biocompatible polyurethane/poly(lactic acid)/GO nanocomposites revealed enhanced anisotropic thermal properties at loadings above the percolation threshold.<sup>262</sup> Graphene nanocomposite membranes had been reported, and their applications in water treatment shown remarkable performance.<sup>263</sup>

A review on biomedically relevant polymers and hydrogels was conducted, emphasizing the role of direct ink writing (DIW) and SLA.<sup>264</sup> Both methods were found to be relevant for 3D printing complex fluids and photoresin compositions.<sup>265–268</sup> Thermo-mechanically enhanced properties were observed in 3D-printed nanocomposites with chitosan-surfactant complexes and chitin nanowhiskers fabricated by SLA.<sup>256,269</sup> It should be noted that polymeric and polyelectrolyte membranes are also pertinent for biomedical applications.<sup>270</sup>

Selective laser sintering (SLS) is another promising option for controlling thermal and electrical conductivity.<sup>271</sup> high-performance polymers (HPP) materials for membranes possess high melting points, chemical resistivity, and specific morphologies that can be adjusted to be more porous or microporous, phase-segregated, to enable selective separation performance.<sup>272</sup> We reported on the importance of reliable mechanical characterization of 3D-printed polymers<sup>273</sup> and its relevance for evaluating HPP.<sup>204,227,229,233</sup> Shape memory properties of thermoset nanocomposites and elastomers were highlighted using carbon nanotubes as a key filler material, based on a modified fused deposition modeling (FDM) method.<sup>131,213</sup>

3D printing for filtration includes water desalination, municipal, water purification, oil-water separation, organic-pollutant removal, gas separation, and nuclear cleanup.<sup>211</sup> Achieving controlled surface wetting is key to anti-fouling, and combining membrane filters with superhydrophobic surfaces has proven highly effective in optimizing performance across diverse separation applications.<sup>274</sup> Following our prior research on anti-corrosion and anti-bacterial surfaces, we subsequently reported the development of parahydrophobic multi-reaction platforms via SLA 3D printing, and showcased the achievement of superhydrophobicity by optimizing SLA slicing parameters and G-code to create non-wetting surface geometries.<sup>275,276</sup> Polyvinylidene fluoride (PVDF) membranes are an important class of semi-crystalline polymers known for their chemical resistance, non-biofouling properties, thermal processability from a relatively low melting point, and piezoelectric behavior.<sup>277</sup> More recently, we have reported on the 3D printing and fabrication of high-performance PVDF parts and sensors.<sup>278–281</sup> In addition, we demonstrated a distinct mechanism for anti-corrosion applications with nylon particle composites, with a swelling-adhesion model to explain this advantage.<sup>282</sup>

As previously mentioned, polyelectrolyte complexes (PEC) and polyelectrolyte multilayers (PEMs) are important membrane materials for controlled ion transport, fuel cell applications, and

small-molecule transport or drug delivery.<sup>7,283,284</sup> PECs and their coacervates tend to precipitate from solution, and possible methods for utilizing PEC as processible, extrudable, or film-forming materials and membranes are through the saloplastics concept.<sup>285,286</sup> We were among the first to report the 3D printing of these saloplastics in air by DIW, enabled by their controlled rheology and in situ conversion to solid-state form via water flushing. These formulated PECs were rheologically optimized for extrusion, enabling us to build objects via 3D printing.<sup>268</sup> A follow-up work demonstrated the 3D printing of these PECs through the addition of silica particles, which did not necessitate the flushing method.<sup>267</sup> Incorporating PECs into photopolymerizable resins via SLA 3D printing demonstrated photocurable, variable small-molecule diffusion properties in hydrogels with future membrane applications.<sup>265</sup> SLA 3D-printing of PEGMA-co-(PNIPAM crosslinked with PEGDA) hydrogels also showed controlled diffusion and swelling behavior.<sup>266</sup>

Vitrimers are another interesting class of polymers due to their dynamic bond properties and recyclability.<sup>287-289</sup> These polymers facilitate dynamic cross-linking and the continuous exchange of covalent and non-covalent bonds, yielding robust, flexible, and solvent-resistant films and membranes. Various membrane applications of vitrimers have been reported, highlighting these advantages.<sup>287,288,290</sup> Building on our work in vitrimeric materials, we successfully engineered a 3D-printable polyurea vitrimeric elastomer, which not only provides a pathway for mechanically isotropic, recyclable structures but also demonstrates robust self-healing behavior.<sup>291</sup> We also developed a 3D-printable, exceptionally tough, and recyclable vitrimeric PDMS elastomer that utilizes a rational network design to produce an elastic network (REN) with optimized rheological behavior.<sup>289</sup> A novel thioctic acid (TA)-based dynamic bond polymerization was recently reported, featuring disulfide linkages and 3D printing.<sup>292</sup>

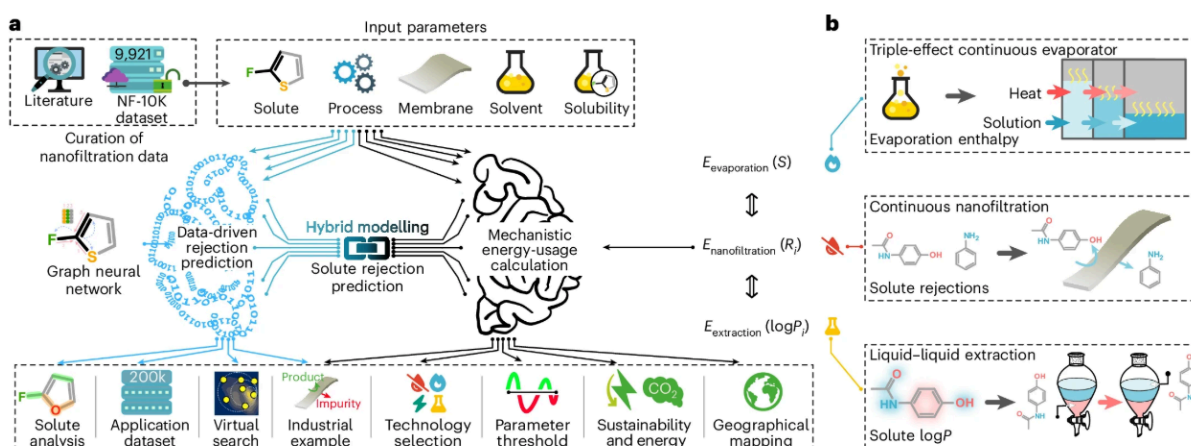
In addition, we developed a 3D-printable carbonated cementitious material (CMM), which demonstrates effective CO<sub>2</sub> gas-diffusion while simultaneously improving the thermo-mechanical properties of the resulting structures.<sup>293</sup>

## 8. Fluidics and Autonomous Self-driving Labs for Membrane Research

With the introduction of self-driving laboratories, high-throughput experimentation (HTE) can be deployed for membrane polymer synthesis and characterization.<sup>294–296</sup> The high-throughput arraying of multivariate analysis and the generation of optimized data for further training, augmented by ML-driven design and algorithms, will be a game-changer. (Figure 9) Proxy experiments or scaled-down experiments can be done with smaller quantities or samples of materials.<sup>294–297</sup>

The increasing interest in self-driving laboratories (SDLs) underscores their potential to revolutionize materials synthesis and characterization. By aligning these processes with AI/ML workflows, SDLs offer a scalable approach to accelerate discovery and data-driven material optimization.<sup>298</sup> Research conducted by our group at ORNL utilized machine intelligence to automate the study of functional thin-film materials; by coupling thin-film array fabrication with automated surface-sensitive techniques (acoustic, spectroscopic, microscopic, and dielectric), we demonstrated a scalable, intelligence-centered approach to materials characterization.<sup>299</sup>

By constructing AI/ML-driven SDLs and using continuous flow chemistry (CFC) it will be possible to codify materials discovery in polymers and membranes within the broader AI in science and data ecosystem.<sup>29,300,301</sup> Although still within the realm of chemistry and materials synthesis, the concepts can be translational towards permeability and transport phenomena investigation under flow.<sup>302–304</sup>



**Figure 9.** a, Hybrid modelling for the chemical separation industry. The curated NF-10K dataset was used in the machine learning and energy models to forecast the applicability of nanofiltration in the untapped chemical space (that is, unexplored separations). The eight

implications and results of the hybrid modelling are expected to aid industrial separation design and decision-making.  $E_{\text{evaporation}}$ , energy of evaporation;  $E_{\text{nanofiltration}}$ , energy of nanofiltration;  $E_{\text{extraction}}$ , energy of extraction;  $S$ , solvent;  $R$ , rejection;  $\log P$ , log partition coefficient. **b**, The three chemical separation technologies considered in this research: triple-effect continuous evaporator, continuous nanofiltration and liquid–liquid extraction. (Figure and caption from reference<sup>305</sup> with slight rephrases under a CC BY license 4.0<sup>58</sup>)

ML-driven microfluidic and millifluidic design and control for membranes and transport research is also a growing field.<sup>306</sup> It presents opportunities to miniaturize, as well as to combine theories of membrane transport with those of microfluidics.<sup>307</sup> These miniaturized devices can be used to study membrane and filtration processes. It can model permeability at scales from nm to mm to represent various porous media in NF and UF. In-situ and real-time studies with microscopy, high-speed imaging, and spectroscopy can model various membrane and filtration processes.<sup>308</sup> The fabrication of membranes and incorporation with microfluidics is a challenge, but with many potential applications for ion transport, separations, biology, drug delivery, and sensing.<sup>307</sup> An SDL in microfluidics or millifluidics for membrane research can enable more complex statistical models or ML-directed algorithms trained for pattern recognition and event prediction in microfluidics.<sup>309</sup> The fluidics research at this scale can implement more ML-directed design and validation via HTE. This can also be enhanced through 3D printing for prototyping devices in fields such as capillary electrophoresis, metal nanoparticle synthesis, aerofluidics, and perovskite nanocrystals.<sup>310</sup> Materials synthesis is the current emphasis on SDL and can also be turned to permeability and selectivity testing.<sup>311–316</sup> High-throughput characterization with real-time spectra and high-speed imaging has been established for online optical control in microfluidics.<sup>317</sup> Drop microfluid agents (DMFAs) for an autonomous droplet microfluidic system are suitable for LLM agent deployment.<sup>318</sup>

HTE-driven SDLs effectively bridge the gap between AI-driven design and membrane performance simulation. By facilitating MI-validated experiments on selectivity and permeability—specifically within varied packed-bed and porous-flow supports—this framework enhances our understanding of transport behavior, hydrodynamics, and multiphase reaction dynamics.<sup>319</sup> This implementation contributes significantly to data analytics and agentic AI for membrane research. Adherence to FAIR data principles enables high-quality, standardized datasets, while reinforcement learning (RL) provides a necessary framework for multi-step, multi-variate optimization—such as chemical environment screening. By leveraging deep reinforcement learning (DRL) for hyperparameter tuning, we can achieve self-optimizing

discovery loops. Establishing an HTE-SDL pipeline is the critical prerequisite for realizing this level of autonomous, bench-scale materials research.

Continuous flow chemistry (CFC) and microreactor technologies offer scalable, modular alternatives to batch processing, providing superior precision in fluidic control and automation. While traditionally utilized for organic synthesis and the fabrication of polymers and nanomaterials, CFC platforms are uniquely suited for dedicated permeability and selectivity testing in pressurized environments. Current research focuses on advancing these platforms into High-Throughput Experimentation (HTE) stations integrated with autonomous Self-Driving Laboratory (SDL) capabilities. We aim to implement modular packed-bed column architectures with precise control over gas-liquid inputs, ultimately enabling AI/ML-optimized workflows for next-generation membrane and permeability research.

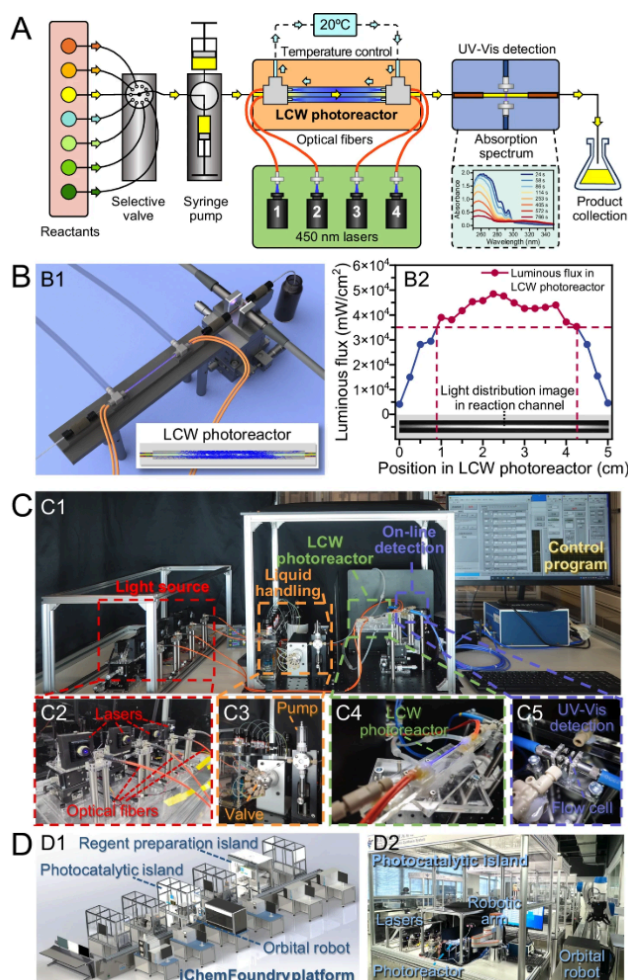


Figure 10. A Schematic diagram of the system flow manifold. B Structure and light distribution of the LCW photocatalytic microreactor. (B1) Schematic diagram of the LCW photocatalytic microreactor and online UV-Vis absorption spectroscopic detection device; (B2) Cross-sectional light intensity distribution in the reaction channel of the LCW photocatalytic microreactor obtained using TracePro software. C Photographs of the system. (C1) Overview of the system. (C2) Light source module, consisting of four 450-nm lasers and four optical fibers. (C3) Liquid handling module with a 10-port selective valve and a syringe pump. (C4) LCW photocatalytic microreactor. (C5) Online UV-Vis absorption spectroscopic detection module. D Schematic diagram (D1) and photograph (D2) of the iChemFoundry platform. (Figures and captions from reference<sup>320</sup> with no change under a creative commons BY-NC-ND 4.0 license<sup>125</sup>) LCW refers to liquid-core waveguide.

Some important current examples of AI/ML workflows and integration in high-throughput experimentation, including CFC and reaction optimization, have been demonstrated. Although established for synthesis and reaction engineering, they can be repurposed for membrane research.<sup>320,321</sup> (Figure 10) An autonomous discovery and optimization platform in an SDL setup can be guided by reinforcement learning (RL) and Bayesian optimization.<sup>322,323</sup> For membrane polymer materials, an SDL setup can automate synthesis and test new polymer designs generated by ML-driven simulation. Important questions beyond increasing yield include answering

fundamental questions about sequence polymerization (copolymerization), microstructure control, branching, topological polymer control, macrocycles, etc.<sup>320,324</sup>

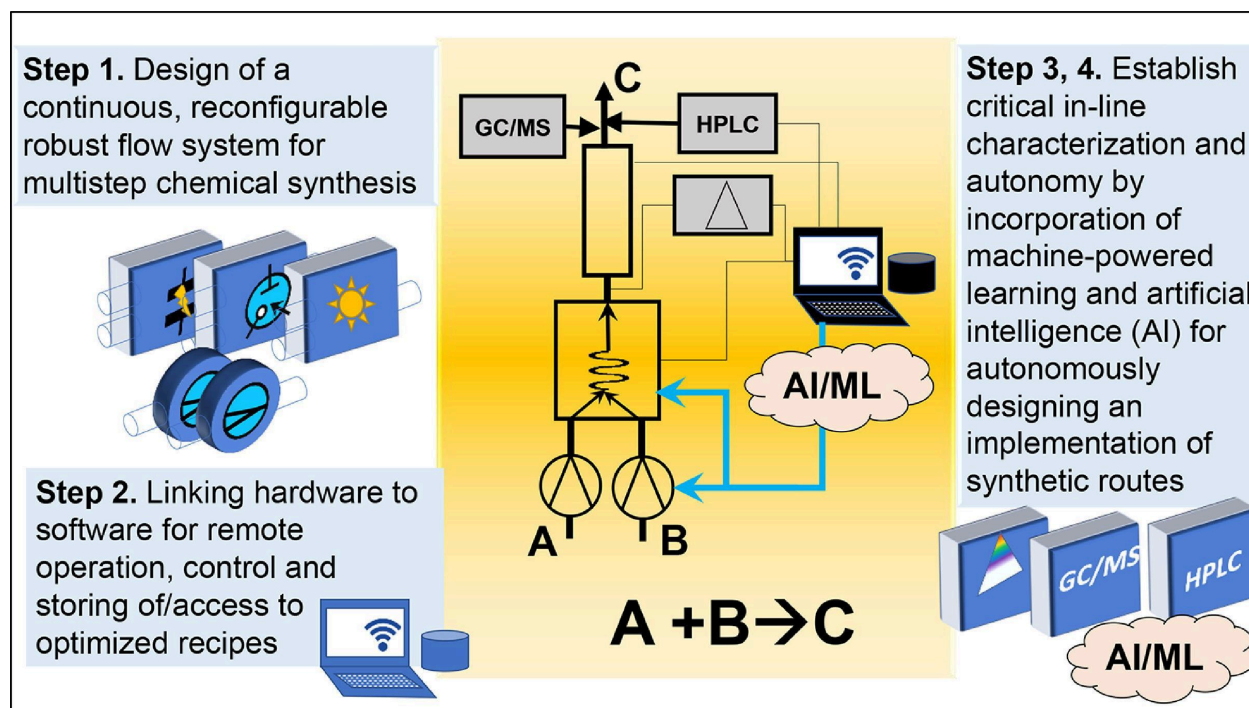


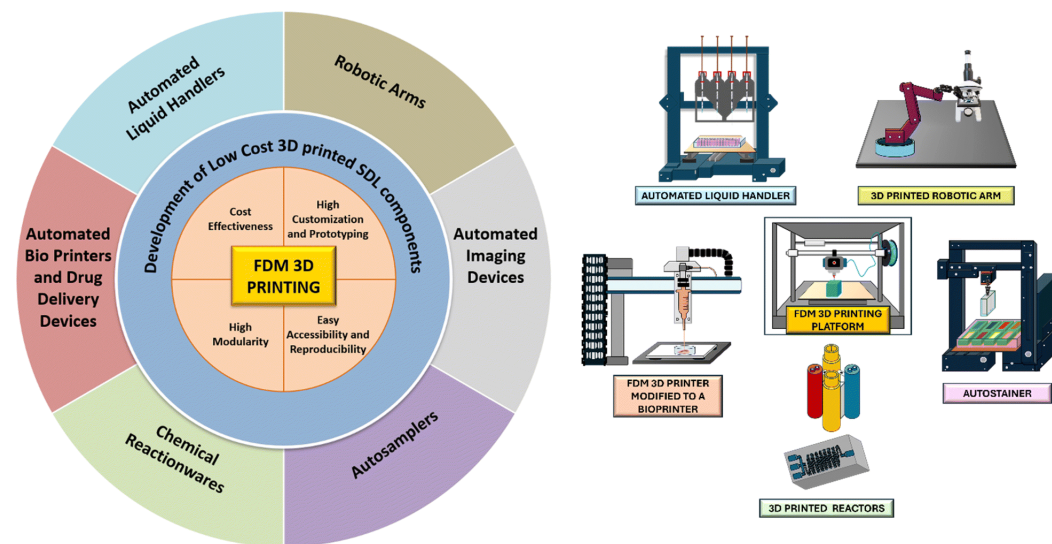
Figure 11. Steps for developing an autonomous continuous flow reactor synthesis for atom-precision with scalability. (Figure and caption from reference<sup>325</sup> with no change under a CC BY-NC-ND 4.0 license<sup>125</sup>)

We previously assessed the feasibility of using autonomous continuous-flow reactors for precision polymerization and scalable material synthesis (Figure 11).<sup>325</sup> Building upon our previous work, we successfully utilized CFC platforms to synthesize block copolymer-grafted silica microparticles using water/ethanol solvent systems.<sup>326</sup> By utilizing a continuous-flow RAFT polymerization process in an ethanol/water solvent system, we achieved superior kinetic control, allowing for the fine-tuning of molecular weight distribution (polydispersity) through precise adjustments in residence time and flow velocity.<sup>327</sup> Leveraging the precise control of continuous flow reactors, we achieved the synthesis of hyperbranched PDMAEMA-grafted silica microparticles via ATRP, showcasing the platform's utility for complex polymer architectures.<sup>328</sup> Additionally, we utilized PET-RAFT polymerization to facilitate the synthesis of hyperbranched architectures through self-condensing vinyl polymerization.<sup>329</sup> A review of the PET-RAFT process for CFC and surface reactions in thin films has been reported.<sup>330</sup>

From CFC, the conversion to SDL methods involves automating the CFC and enabling real-time sensing with feedback on the polymerization process, as well as the ability to control reaction parameters in situ (e.g., flow rate, temperature, pressure, and dosing) to intervene on the reaction and alter the results. SDLs for emulsion polymerization have been previously reported.<sup>331</sup> We have reported on the use of SDLs to address questions in ML-Driven copolymerization and demonstration of feedback loop protocols that also include MD simulation.<sup>301,332</sup>

## Lowering the barrier to SDLs in Membrane research and testing

Ultimately, this framework offers a pathway to democratize high-throughput and autonomous research. (Figure 12) By making these technologies viable at the bench scale, we empower the next generation of scientists with the tools to master complex workflows in materials synthesis and process engineering. Integrating AI/ML-driven workflows allows for the development of bench-scale instrumentation that synthesizes flow chemistry, modular separation units, and mechatronics-based diagnostic testing—all while achieving significant cost-efficiencies compared to traditional research platforms.<sup>333</sup> Configuring the CFC as a packed-bed column enables a simplified, affordable closed-loop station for testing membrane separations and porous-flow performance. This setup is ideally suited for applying statistical DOE and machine-learning-driven optimization to complex reaction engineering workflows.<sup>334</sup> Pressurization or pressure drop measurements will be needed, including more robust tubing and valves. This is augmented by using 3D printing as a CNC movement platform and building CFC parts.<sup>335,336</sup> Microfluidics and millifluidics are appropriate entry points for rapid prototyping and for implementing the principles of transport and separation in micro- to millimeter-scale devices or designs for filtration,<sup>337–339</sup> with open-source interactive design platforms.<sup>340–342</sup>



**Figure 12.** Development of low-cost 3D-printed SDL components: a focus on affordable and accessible solutions for self-driving labs. (Figure and caption from reference<sup>335</sup> with no change under a creative commons license 3.0<sup>10</sup>)

Bridging the gap between advanced research and education, the implementation of 3D-printed, CFC-based stations allows for the democratization of high-throughput experimental training. This approach empowers students to engage with AI-driven, autonomous workflows for membrane fabrication and materials testing at an early stage in their academic careers.<sup>338,343–346</sup> It will be important to introduce robotics, mechatronics, and electronics, including Arduino, Raspberry Pi, IOT electronics.<sup>347</sup> Ultimately, this roadmap facilitates the adoption of autonomous membrane research across diverse settings, from educational labs to small to medium-scale enterprises (SMEs). Integrating democratized HTE and SDL platforms into these environments fosters an accelerated learning curve, training a workforce prepared to leverage AI/ML for the next generation of materials discovery.<sup>171</sup>

## 9. Future Applications

A driving force for future applications of membranes and separations can be end-to-end AI/ML workflows. Knowledge, skills, and investments can be made at specific stages of planning. A good number of these applications are essentially process intensification and address critical needs related to materials supply chains, energy reduction, and health. Here are a few examples:

1. Critical Minerals and Rare Earth Elements (REE) extraction and recovery from tailings, mine wastes, and combustion ash.<sup>348,349</sup>
2. Isotope's enhancement and separations: recovery and separations beyond distillation, water isotope filtration, separation of helium, and lithium isotope separation.<sup>350–352</sup>
3. Biorefining and bioreactors: biofuel production, recycling, pervaporation in solvent and chemical intermediates purification.<sup>353–355</sup>
4. Sensing and molecular separations: Biosensors, stimuli-responsive membranes, new PIM membranes, and hybrid MOF and COF membranes.<sup>356,357</sup>

## 10. CONCLUSION

The integration of end-to-end AI/ML workflows into membrane science offers transformative potential for optimizing separation and filtration processes. Advancing our understanding of diffusion and transport phenomena across multiple length scales is crucial for the development of high-performance polymers and composites. By leveraging inverse design, we can address complex technical challenges across diverse industrial sectors.

Various machine learning algorithms—including linear regression, support vector machines (SVM), decision trees, random forests (RF), and neural networks (NN)—provide powerful tools for modeling membrane performance. These models are instrumental in predicting key figures of

merit, such as selectivity, permeability, rejection rates, and long-term stability across reverse osmosis (RO), nanofiltration (NF), ultrafiltration (UF), and microfiltration (MF) systems. Furthermore, Bayesian optimization enables the precise tuning of operating parameters—including temperature, pressure, flux, and flow rate—to achieve peak efficiency. Such optimization not only maximizes performance but also reduces energy consumption, thereby extending membrane service life and decreasing maintenance requirements. Looking forward, predictive ML-driven models are poised to enhance real-time operations, enabling early fault detection in critical applications such as micropollutant removal, forward osmosis (FO), food and beverage processing, biosystems, and energy management.

Despite this potential, significant challenges persist, including data scarcity, model incompatibility, and the high computational costs of implementation. Overcoming these barriers requires the adoption of autonomous Self-Driving Laboratories (SDLs) and a shift toward collaborative, federated research infrastructures that prioritize standardized data formats. The establishment of reliable, open-access databases for diverse membrane systems is essential to fuel advanced reinforcement learning (RL) and deep learning (DL) architectures. Finally, the proliferation of affordable generative AI and Large Language Model (LLM) tools will improve model interpretability, empowering researchers to better understand the decision-making processes underlying AI predictions. The convergence of these technological advancements signals a promising future for AI-assisted membrane research.

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## Conflicts of Interest

The author declares no conflict of interest. A preprint draft has been deposited in an archive repository, which was not targeted to a specific journal.

## Author Contributions

RCA planned the layout. RCA and JC all contributed to the overall design and writing.

## Reference:

- (1) *Membrane Separations Technology*. ScienceDirect. <http://www.sciencedirect.com:5070/book/monograph/9780750677103/membrane-separations-technology?via=ihub%3D> (accessed 2026-02-04).
- (2) Sholl, D. S.; Lively, R. P. Seven Chemical Separations to Change the World. *Nature* **2016**, 532 (7600), 435–437. <https://doi.org/10.1038/532435a>.
- (3) Robeson, L. M.; Burgoyne, W. F.; Langsam, M.; Savoca, A. C.; Tien, C. F. High Performance Polymers for Membrane Separation. *Polymer* **1994**, 35 (23), 4970–4978. [https://doi.org/10.1016/0032-3861\(94\)90651-3](https://doi.org/10.1016/0032-3861(94)90651-3).
- (4) Mahmud, R.; Moni, S. M.; High, K.; Carbajales-Dale, M. Integration of Techno-Economic Analysis and Life Cycle Assessment for Sustainable Process Design – A Review. *J. Clean. Prod.* **2021**, 317, 128247. <https://doi.org/10.1016/j.jclepro.2021.128247>.
- (5) Kamalesh, R.; Karishma, S.; Saravanan, A.; Yaashikaa, P. R. Emerging Breakthroughs in Membrane Filtration Techniques and Their Application in Agricultural Wastewater Treatment: Reusability Aspects. *Sustain. Chem. Environ.* **2024**, 8, 100183. <https://doi.org/10.1016/j.scenv.2024.100183>.
- (6) MEMBRANE SEPARATIONS | Membrane Preparation. **2000**, 1755–1764. <https://doi.org/10.1016/B0-12-226770-2/05241-8>.
- (7) Avneri, B.; Li, K.; Stolov, M.; Ulbricht, M.; Freger, V. Polyelectrolyte-Ionomer Complex Nanofiltration Membranes: Complexation Stoichiometry, Kinetics, and Separation Performance. *J. Membr. Sci.* **2025**, 735, 124510. <https://doi.org/10.1016/j.memsci.2025.124510>.
- (8) Grunlan, M. A.; Korley, L. T. J.; Lin, Q.; Soles, C. L.; Advincula, R.; Jayaraman, A.; Cosgriff-Hernandez, E.; Reichmanis, E.; Lutkenhaus, J. L.; Priestley, R. D.; Voit, B.; Epps, T. H. I. PMSE Centennial: Celebration of Success and New Frontiers in Polymer Materials Science and Engineering. *ACS Macro Lett.* **2025**, 14 (10), 1465–1475. <https://doi.org/10.1021/acsmacrolett.5c00626>.
- (9) Comesaña-Gándara, B.; Chen, J.; Bezzu, C. G.; Carta, M.; Rose, I.; Ferrari, M.-C.; Esposito, E.; Fuoco, A.; Jansen, J. C.; McKeown, N. B. Redefining the Robeson Upper Bounds for CO<sub>2</sub>/CH<sub>4</sub> and CO<sub>2</sub>/N<sub>2</sub> Separations Using a Series of Ultrapermeable

- Benzotriptycene-Based Polymers of Intrinsic Microporosity. *Energy Environ. Sci.* **2019**, *12* (9), 2733–2740. <https://doi.org/10.1039/C9EE01384A>.
- (10) Deed - Attribution 3.0 Unported - Creative Commons. <https://creativecommons.org/licenses/by/3.0/> (accessed 2026-01-15).
- (11) *Advanced Polymeric Nanocomposite Membranes for Water and Wastewater Treatment: A Comprehensive Review*. <https://www.mdpi.com/2073-4360/15/3/540> (accessed 2026-02-04).
- (12) McKeown, N. B.; Budd, P. M. Polymers of Intrinsic Microporosity (PIMs): Organic Materials for Membrane Separations, Heterogeneous Catalysis and Hydrogen Storage. *Chem. Soc. Rev.* **2006**, *35* (8), 675–683. <https://doi.org/10.1039/B600349D>.
- (13) Adeola, A. O.; Nomngongo, P. N. Advanced Polymeric Nanocomposites for Water Treatment Applications: A Holistic Perspective. *Polymers* **2022**, *14* (12), 2462. <https://doi.org/10.3390/polym14122462>.
- (14) Kancherla, R.; Nazia, S.; Kalyani, S.; Sridhar, S. Modeling and Simulation for Design and Analysis of Membrane-Based Separation Processes. *Comput. Chem. Eng.* **2021**, *148*, 107258. <https://doi.org/10.1016/j.compchemeng.2021.107258>.
- (15) Nistane, J.; Datta, R.; Lee, Y. J.; Sahu, H.; Jang, S. S.; Lively, R.; Ramprasad, R. Polymer Design for Solvent Separations by Integrating Simulations, Experiments and Known Physics via Machine Learning. *Npj Comput. Mater.* **2025**, *11* (1), 187. <https://doi.org/10.1038/s41524-025-01681-8>.
- (16) Ma, R.; Li, J.; Zeng, P.; Duan, L.; Dong, J.; Ma, Y.; Yang, L. The Application of Membrane Separation Technology in the Pharmaceutical Industry. *Membranes* **2024**, *14* (1). <https://doi.org/10.3390/membranes14010024>.
- (17) Li, J.; Li, L.; Brink, H. A.; Allegri, G.; Lindhoud, S. Polyelectrolyte Complex-Based Materials for Separations: Progress, Challenges and Opportunities. *Mater. Horiz.* **2025**, *12* (14), 4998–5030. <https://doi.org/10.1039/D4MH01840K>.
- (18) Tian, L.; Duan, H.; Luo, J.; Cheng, Y.; Shi, L. Density Functional Theory and Molecular Dynamics Simulations of Nanoporous Graphene Membranes for Hydrogen Separation. *ACS Appl. Nano Mater.* **2021**, *4* (9), 9440–9448. <https://doi.org/10.1021/acsnm.1c01919>.
- (19) Mollahosseini, A.; Abdelrasoul, A. Molecular Dynamics Simulation for Membrane Separation and Porous Materials: A Current State of Art Review. *J. Mol. Graph. Model.* **2021**, *107*, 107947. <https://doi.org/10.1016/j.jmgm.2021.107947>.
- (20) Li, X.; Jiang, F.; Ravindra, A. V.; Zhou, J.; Zhou, A.; Le, T.; Peng, J.; Ju, S. Mixing Processes in a 3D Printed Large-Flow Microstructured Reactor: Finite Element Simulations and Experimental Study. *Chem. Eng. J.* **2019**, *370*, 295–304. <https://doi.org/10.1016/j.cej.2019.03.187>.
- (21) Szabó, B.; Babuška, I. *Finite Element Analysis: Method, Verification and Validation*; John Wiley & Sons, 2021.
- (22) Jafari, M.; Tzirtzipi, C.; Castro-Dominguez, B. Applications of Artificial Intelligence for Membrane Separation: A Review. *J. Water Process Eng.* **2024**, *68*, 106532. <https://doi.org/10.1016/j.jwpe.2024.106532>.
- (23) *A Survey of AI for Materials Science: Foundation Models, LLM Agents, Datasets, and Tools*. <https://arxiv.org/html/2506.20743v1> (accessed 2026-01-13).
- (24) Werheid, J.; Melnychuk, O.; Zhou, H.; Huber, M.; Rippe, C.; Joosten, D.; Keskin, Z.; Wittstamm, M.; Subramani, S.; Drescher, B.; Göppert, A.; Abdelrazeq, A.; Schmitt, R. H.

- Designing an LLM-Based Copilot for Manufacturing Equipment Selection. *Manuf. Lett.* **2025**, *46*, 123–127. <https://doi.org/10.1016/j.mfglet.2025.10.017>.
- (25) Advincula, R.; Chen, J. Advanced Manufacturing with Renewable and Bio-Based Materials: AI/ML Workflows and Process Optimization. arXiv January 15, 2026. <https://doi.org/10.48550/arXiv.2601.10382>.
- (26) Chen, J.; Yuan, Y.; Wang, Q.; Wang, H.; Advincula, R. C. Bridging Additive Manufacturing and Electronics Printing in the Age of AI. *Nanomaterials* **2025**, *15* (11), 843. <https://doi.org/10.3390/nano15110843>.
- (27) Chen, J.; Advincula, R. Artificial Intelligence in Advanced Polymer Manufacturing. *Engineering Archive* January 15, 2026. <https://doi.org/10.31224/6281>.
- (28) Chen, J.; Christakopoulos, P.; Ivanov, I. N.; Vasudevan, R. K.; Kumar, R.; Sumpter, B. G.; Advincula, R. C. Artificial Intelligence/Machine Learning of Polymer Materials and Discovery Chemistry. *MRS Bull.* **2025**, *50* (11), 1364–1375. <https://doi.org/10.1557/s43577-025-00986-9>.
- (29) Chen, J.; Yuan, Y.; Ziabari, A. K.; Xu, X.; Zhang, H.; Christakopoulos, P.; Bonnesen, P. V.; Ivanov, I. N.; Ganesh, P.; Wang, C.; Jaimes, K. P.; Yang, G.; Kumar, R.; Sumpter, B. G.; Advincula, R. AI for Manufacturing and Healthcare: A Chemistry and Engineering Perspective. arXiv May 2, 2024. <https://doi.org/10.48550/arXiv.2405.01520>.
- (30) Chen, J.; Christakopoulos, P.; Chen, K. D.; Ivanov, I. N.; Advincula, R. Agentic AI and Machine Learning for Accelerated Materials Discovery and Applications. arXiv January 15, 2026. <https://doi.org/10.48550/arXiv.2601.09027>.
- (31) Wang, X. Q.; Jin, Z.; Ravichandran, D.; Gu, G. X. Artificial Intelligence and Multiscale Modeling for Sustainable Biopolymers and Bioinspired Materials. *Adv. Mater.* **2025**, *37* (22), 2416901. <https://doi.org/10.1002/adma.202416901>.
- (32) Bernardes, A. F.; Meng, Z.; Campos, L. C.; Coppens, M.-O. Bio-Inspired Anti-Fouling Strategies for Membrane-Based Separations. *Chem. Commun.* **2025**, *61* (27), 5064–5071. <https://doi.org/10.1039/D4CC05149A>.
- (33) Dangayach, R.; Jeong, N.; Demirel, E.; Uzal, N.; Fung, V.; Chen, Y. Machine Learning-Aided Inverse Design and Discovery of Novel Polymeric Materials for Membrane Separation. *Environ. Sci. Technol.* **2025**, *59* (2), 993–1012. <https://doi.org/10.1021/acs.est.4c08298>.
- (34) Ritt, C. L.; Quien, M.; Wei, Z.; Gress, H.; Dronadula, M. T.; Altmisdort, K.; Nguyen, H. G. T.; Zangmeister, C. D.; Tu, Y.-M.; Garimella, S. S.; Amirabadi, S.; Gadaloff, M.; Hu, W.; Aluru, N. R.; Ekinci, K. L.; Bunch, J. S.; Strano, M. S. A Molecularly Impermeable Polymer from Two-Dimensional Polyaramids. *Nature* **2025**, *647* (8089), 383–389. <https://doi.org/10.1038/s41586-025-09674-9>.
- (35) Osman, A. I.; Nasr, M.; Farghali, M.; Bakr, S. S.; Eltaweil, A. S.; Rashwan, A. K.; Abd El-Monaem, E. M. Machine Learning for Membrane Design in Energy Production, Gas Separation, and Water Treatment: A Review. *Environ. Chem. Lett.* **2024**, *22* (2), 505–560. <https://doi.org/10.1007/s10311-023-01695-y>.
- (36) Viet, N. D.; Jang, D.; Yoon, Y.; Jang, A. Enhancement of Membrane System Performance Using Artificial Intelligence Technologies for Sustainable Water and Wastewater Treatment: A Critical Review. *Crit. Rev. Environ. Sci. Technol.* **2022**, *52* (20), 3689–3719. <https://doi.org/10.1080/10643389.2021.1940031>.

- (37) Dmitrieva, E. S.; Anokhina, T. S.; Novitsky, E. G.; Volkov, V. V.; Borisov, I. L.; Volkov, A. V. Polymeric Membranes for Oil-Water Separation: A Review. *Polymers* **2022**, *14* (5), 980. <https://doi.org/10.3390/polym14050980>.
- (38) Hadi, M. K.; Wang, X.; Peng, Y.; Sangaraju, S.; Ran, F. Functional Polymeric Membrane Materials: A Perspective from Versatile Methods and Modification to Potential Applications. *Polym. Sci. Technol.* **2025**, *1* (5), 366–412. <https://doi.org/10.1021/polymstech.4c00030>.
- (39) Karki, S.; Hazarika, G.; Yadav, D.; Ingole, P. G. Polymeric Membranes for Industrial Applications: Recent Progress, Challenges and Perspectives. *Desalination* **2024**, *573*, 117200. <https://doi.org/10.1016/j.desal.2023.117200>.
- (40) *A Review on Porous Polymeric Membrane Preparation. Part II: Production Techniques with Polyethylene, Polydimethylsiloxane, Polypropylene, Polyimide, and Polytetrafluoroethylene.* <https://www.mdpi.com/2073-4360/11/8/1310> (accessed 2026-02-04).
- (41) Hameed, M. U.; Ali, L.; Ahmad, A.; Zhang, P.; Raza, S.; Khan, S.; Liu, W.-R.; Amjad, Z. Recent Progress in Biomass Polymer Based Hydrogel Membranes for Adsorption and Photocatalytic Pollutants Removal: Fabrication, Challenges and Future Perspectives. *Desalination* **2025**, *615*, 119216. <https://doi.org/10.1016/j.desal.2025.119216>.
- (42) Ben Dassi, R.; Chamam, B. Nanomaterial-Enhanced Membranes for Advanced Water and Wastewater Treatment: A Comprehensive Review. *Rev. Environ. Sci. Biotechnol.* **2025**, *24* (2), 477–511. <https://doi.org/10.1007/s11157-025-09723-9>.
- (43) Fuseini, M.; El-Shazly, A. H.; Zaghloul, M. M. Y. Recent Progress in Membrane Engineering: Advanced Materials and Manufacturing Techniques. *Polym. Adv. Technol.* **2025**, *36* (12), e70468. <https://doi.org/10.1002/pat.70468>.
- (44) Gough, C. R.; Callaway, K.; Spencer, E.; Leisy, K.; Jiang, G.; Yang, S.; Hu, X. Biopolymer-Based Filtration Materials. *ACS Omega* **2021**, *6* (18), 11804–11812. <https://doi.org/10.1021/acsomega.1c00791>.
- (45) More, N.; Avhad, M.; Utekar, S.; More, A. Polylactic Acid (PLA) Membrane—Significance, Synthesis, and Applications: A Review. *Polym. Bull.* **2023**, *80* (2), 1117–1153. <https://doi.org/10.1007/s00289-022-04135-z>.
- (46) Islam, M. S.; Elahee, G. M. F.; Fang, Y.; Yu, X. (Bill); Advincula, R. C.; Cao, C. (Chase). Polylactic Acid (PLA)-Based Multifunctional and Biodegradable Nanocomposites and Their Applications. *Compos. Part B Eng.* **2025**, *306*, 112842. <https://doi.org/10.1016/j.compositesb.2025.112842>.
- (47) Ma, Y.; Zhao, X.; He, B. Fabrication of Nanoparticle Array Membranes by Integrating Semi-Crystalline Polymer Self-Assembly with NIPS for Water Treatment. *Nanoscale Adv.* **2024**, *6* (14), 3543–3552. <https://doi.org/10.1039/D3NA01157G>.
- (48) Yu, S.; Chen, Y.; Qiao, Z.; Hou, J. Processable Microporous Membranes: Emerging Platforms for Separation Technologies. *Chem. Soc. Rev.* **2026**. <https://doi.org/10.1039/D5CS00543D>.
- (49) Shi, Y.; Ilic, O.; Atwater, H. A.; Greer, J. R. All-Day Fresh Water Harvesting by Microstructured Hydrogel Membranes. *Nat. Commun.* **2021**, *12* (1), 2797. <https://doi.org/10.1038/s41467-021-23174-0>.
- (50) *Polymeric Based Hydrogel Membranes for Biomedical Applications.* <https://www.mdpi.com/2077-0375/13/6/576> (accessed 2026-02-04).

- (51) Nocheseda, C. J. C.; Liza, F. P.; Collera, A. K. M.; Caldona, E. B.; Advincula, R. C. 3D Printing of Metals Using Biodegradable Cellulose Hydrogel Inks. *Addit. Manuf.* **2021**, *48*, 102380. <https://doi.org/10.1016/j.addma.2021.102380>.
- (52) Lu, X.; Elimelech, M. Fabrication of Desalination Membranes by Interfacial Polymerization: History, Current Efforts, and Future Directions. *Chem. Soc. Rev.* **2021**, *50* (11), 6290–6307. <https://doi.org/10.1039/D0CS00502A>.
- (53) Theodorakopoulos, G. V.; Karousos, D. S.; Favvas, E. P.; Gotzias, A. D. Formation of Polyimide Membranes via Non-Solvent Induced Phase Separation: Insight from Molecular Dynamics Simulations. *ChemPlusChem* **2024**, *89* (8), e202300766. <https://doi.org/10.1002/cplu.202300766>.
- (54) Greiner, A.; Wendorff, J. H. Electrospinning: A Fascinating Method for the Preparation of Ultrathin Fibers. *Angew. Chem. Int. Ed.* **2007**, *46* (30), 5670–5703. <https://doi.org/10.1002/anie.200604646>.
- (55) Kaya, D.; Keçeci, K. Review—Track-Etched Nanoporous Polymer Membranes as Sensors: A Review. *J. Electrochem. Soc.* **2020**, *167* (3), 037543. <https://doi.org/10.1149/1945-7111/ab67a7>.
- (56) Nunes, S. P.; Culfaz-Emecen, P. Z.; Ramon, G. Z.; Visser, T.; Koops, G. H.; Jin, W.; Ulbricht, M. Thinking the Future of Membranes: Perspectives for Advanced and New Membrane Materials and Manufacturing Processes. *J. Membr. Sci.* **2020**, *598*, 117761. <https://doi.org/10.1016/j.memsci.2019.117761>.
- (57) Hays, S. S.; Pokorski, J. K. Solvent-Free Membrane Manufacturing via Melt Processing. *Curr. Opin. Chem. Eng.* **2025**, *47*, 101061. <https://doi.org/10.1016/j.coche.2024.101061>.
- (58) Deed - Attribution 4.0 International - Creative Commons. <https://creativecommons.org/licenses/by/4.0/> (accessed 2025-03-19).
- (59) Ismail, A. F.; Khulbe, K. C.; Matsuura, T. Membrane Fabrication/Manufacturing Techniques. In *Gas Separation Membranes: Polymeric and Inorganic*; Ismail, A. F., Chandra Khulbe, K., Matsuura, T., Eds.; Springer International Publishing: Cham, 2015; pp 193–220. [https://doi.org/10.1007/978-3-319-01095-3\\_4](https://doi.org/10.1007/978-3-319-01095-3_4).
- (60) Zhu, Y.; Booth, A. J.; Eatman, J. G.; Kim, M. A.; Liu, Y.; Sarkar, B.; Sengupta, B.; Yue, X.; Amanchukwu, C. V.; Darling, S. B.; Elam, J. W.; Fenter, P.; Liu, C.; Hatzell, K. B. From Molecules to Modules: Advanced Characterization of Membrane Systems. *Adv. Mater.* **2026**, *38* (1), e13056. <https://doi.org/10.1002/adma.202513056>.
- (61) Alqaheem, Y.; Alomair, A. A. Microscopy and Spectroscopy Techniques for Characterization of Polymeric Membranes. *Membranes* **2020**, *10* (2), 33. <https://doi.org/10.3390/membranes10020033>.
- (62) Mehta, A.; Zydney, A. L. Permeability and Selectivity Analysis for Ultrafiltration Membranes. *J. Membr. Sci.* **2005**, *249* (1), 245–249. <https://doi.org/10.1016/j.memsci.2004.09.040>.
- (63) Lee, Y. J.; Chen, L.; Nistane, J.; Jang, H. Y.; Weber, D. J.; Scott, J. K.; Rangnekar, N. D.; Marshall, B. D.; Li, W.; Johnson, J. R.; Bruno, N. C.; Finn, M. G.; Ramprasad, R.; Lively, R. P. Data-Driven Predictions of Complex Organic Mixture Permeation in Polymer Membranes. *Nat. Commun.* **2023**, *14* (1), 4931. <https://doi.org/10.1038/s41467-023-40257-2>.
- (64) Xu, Q.; Jiang, J. Molecular Simulations of Liquid Separations in Polymer Membranes. *Curr. Opin. Chem. Eng.* **2020**, *28*, 66–74. <https://doi.org/10.1016/j.coche.2020.02.001>.

- (65) Ramanamane, N.; Pita, M.; Sob, B. Advanced Low–Cost Natural Materials for High–Performance Oil–Water Filtration Membranes: Achievements, Challenges, and Future Directions. *Membranes* **2024**, *14* (12). <https://doi.org/10.3390/membranes14120264>.
- (66) Chisca, S.; Musteata, V.-E.; Zhang, W.; Vasylevskiy, S.; Falca, G.; Abou-Hamad, E.; Emwas, A.-H.; Altunkaya, M.; Nunes, S. P. Polytriazole Membranes with Ultrathin Tunable Selective Layer for Crude Oil Fractionation. *Science* **2022**, *376* (6597), 1105–1110. <https://doi.org/10.1126/science.abm7686>.
- (67) Bruno, N. C.; Mathias, R.; Lee, Y. J.; Zhu, G.; Ahn, Y.-H.; Rangnekar, N. D.; Johnson, J. R.; Hoy, S.; Bechis, I.; Tarzia, A.; Jelfs, K. E.; McCool, B. A.; Lively, R.; Finn, M. G. Solution-Processable Polytriazoles from Spirocyclic Monomers for Membrane-Based Hydrocarbon Separations. *Nat. Mater.* **2023**, *22* (12), 1540–1547. <https://doi.org/10.1038/s41563-023-01682-2>.
- (68) Li, S.; Dong, R.; Musteata, V.-E.; Kim, J.; Rangnekar, N. D.; Johnson, J. R.; Marshall, B. D.; Chisca, S.; Xu, J.; Hoy, S.; McCool, B. A.; Nunes, S. P.; Jiang, Z.; Livingston, A. G. Hydrophobic Polyamide Nanofilms Provide Rapid Transport for Crude Oil Separation. *Science* **2022**, *377* (6614), 1555–1561. <https://doi.org/10.1126/science.abq0598>.
- (69) Zhai, H. Advanced Membranes and Learning Scale Required for Cost-Effective Post-Combustion Carbon Capture. *iScience* **2019**, *13*, 440–451. <https://doi.org/10.1016/j.isci.2019.03.006>.
- (70) Bai, R.; Song, X.; Yan, W.; Yu, J. Low-Energy Adsorptive Separation by Zeolites. *Natl. Sci. Rev.* **2022**, *9* (9), nwac064. <https://doi.org/10.1093/nsr/nwac064>.
- (71) Bazyar, H.; van de Beek, N.; Lammertink, R. G. H. Liquid-Infused Membranes with Oil-in-Water Emulsions. *Langmuir* **2019**, *35* (29), 9513–9520. <https://doi.org/10.1021/acs.langmuir.9b01055>.
- (72) Dar, A. A.; Chen, Z.; Zhang, G.; Hu, J.; Zaghbi, K.; Deng, S.; Wang, X.; Haghghat, F.; Mulligan, C. N.; An, C.; Ramirez, A. A.; Sun, S. Sustainable Extraction of Critical Minerals from Waste Batteries: A Green Solvent Approach in Resource Recovery. *Batteries* **2025**, *11* (2). <https://doi.org/10.3390/batteries11020051>.
- (73) Ge, R.; Huo, T.; Gao, Z.; Li, J.; Zhan, X. GO-Based Membranes for Desalination. *Membranes* **2023**, *13* (2). <https://doi.org/10.3390/membranes13020220>.
- (74) Lakshmy, K. S.; Lal, D.; Nair, A.; Babu, A.; Das, H.; Govind, N.; Dmitrenko, M.; Kuzminova, A.; Korniak, A.; Penkova, A.; Tharayil, A.; Thomas, S. Pervaporation as a Successful Tool in the Treatment of Industrial Liquid Mixtures. *Polymers* **2022**, *14* (8). <https://doi.org/10.3390/polym14081604>.
- (75) Advanced Oil Spill Decontamination Techniques. In *Interface Science and Technology*; Elsevier, 2019; Vol. 30, pp 283–332. <https://doi.org/10.1016/B978-0-12-814178-6.00012-1>.
- (76) Han, Z.; Huang, L.; Qu, H.; Wang, Y.; Zhang, Z.; Rong, Q.; Sang, Z.; Wang, Y.; Kipper, M. J.; Tang, J. A Review of Performance Improvement Strategies for Graphene Oxide-Based and Graphene-Based Membranes in Water Treatment. *J. Mater. Sci.* **2021**, *56* (16), 9545–9574. <https://doi.org/10.1007/s10853-021-05873-7>.
- (77) Advincula, R. C. Superhydrophobic and Nanostructured HPHT Stable Polybenzoxazine Nanocomposite Coatings for Oil and Gas.
- (78) Asrafali, S. P.; Periyasamy, T.; Bari, G. A. K. M. R.; Lee, J. Properties of Polybenzoxazine-Based Conducting Materials in Energy-Related Applications. *Polymers* **2025**, *17* (16), 2194. <https://doi.org/10.3390/polym17162194>.

- (79) Tian, L.; Wang, M.; Liao, G.; Sun, Y.; Chen, Y.; Hu, Y.; Lu, Z. Highly Sulfonated Polybenzoxazine Proton Exchange Membrane with Dimensional Stability and Low Hydrogen Permeability for Water Electrolysis. *Chem. Eng. J.* **2025**, *517*, 164596. <https://doi.org/10.1016/j.cej.2025.164596>.
- (80) Su, P.-K.; Chang, C.-H.; Sun, Y.-M.; Hu, C.-C.; Lai, J.-Y.; Liu, Y.-L. Porous Membranes of Thermosetting Polybenzoxazine Resins with Interconnected-Pores for Organic Solvent Microfiltration. *J. Membr. Sci.* **2019**, *586*, 267–273. <https://doi.org/10.1016/j.memsci.2019.05.061>.
- (81) Caldoná, E. B.; De Leon, A. C. C.; Thomas, P. G.; Naylor, D. F. I.; Pajarito, B. B.; Advincula, R. C. Superhydrophobic Rubber-Modified Polybenzoxazine/SiO<sub>2</sub> Nanocomposite Coating with Anticorrosion, Anti-Ice, and Superoleophilicity Properties. *Ind. Eng. Chem. Res.* **2017**, *56* (6), 1485–1497. <https://doi.org/10.1021/acs.iecr.6b04382>.
- (82) Caldoná, E. B.; de Leon, A. C. C.; Pajarito, B. B.; Advincula, R. C. Novel Anti-Corrosion Coatings from Rubber-Modified Polybenzoxazine-Based Polyaniline Composites. *Appl. Surf. Sci.* **2017**, *422*, 162–171. <https://doi.org/10.1016/j.apsusc.2017.05.083>.
- (83) de Souza, L. R.; d'Almeida, J. R. M.; Cheng, X.; Rong, L.-H.; Caldoná, E. B.; Advincula, R. C. Highly Thermally Stable Copolymers of Epoxy and Trifunctional Polybenzoxazine. *Mater. Today Commun.* **2022**, *30*, 102988. <https://doi.org/10.1016/j.mtcomm.2021.102988>.
- (84) Caldoná, E. B.; De Leon, A. C. C.; Pajarito, B. B.; Advincula, R. C. A Review on Rubber-Enhanced Polymeric Materials. *Polym. Rev.* **2017**, *57* (2), 311–338. <https://doi.org/10.1080/15583724.2016.1247102>.
- (85) Chen, Q.; de Leon, A.; Advincula, R. C. Inorganic–Organic Thiol–Ene Coated Mesh for Oil/Water Separation. *ACS Appl. Mater. Interfaces* **2015**, *7* (33), 18566–18573. <https://doi.org/10.1021/acsami.5b04980>.
- (86) Silva, Í. G. M. da; Lucas, E. F.; Advincula, R. Highly Efficient Oil/Water and Brine Separations: Superhydrophobic Hybrid Isobornyl Methacrylate Coatings. *Sep. Purif. Technol.* **2021**, *278*, 119365. <https://doi.org/10.1016/j.seppur.2021.119365>.
- (87) da Silva, Í. G. M.; Lucas, E. F.; Advincula, R. Fluorine-Free Superhydrophobic Coatings: Rapid Fabrication and Highly Efficient Oil/Water Separation. *Macromol. Mater. Eng.* **2020**, *305* (12), 2000400. <https://doi.org/10.1002/mame.202000400>.
- (88) Conducting Polymers with Superhydrophobic Effects as Anticorrosion Coating. In *Intelligent Coatings for Corrosion Control*; Butterworth-Heinemann, 2015; pp 409–430. <https://doi.org/10.1016/B978-0-12-411467-8.00011-8>.
- (89) Frau, A. F.; Pernites, R. B.; Advincula, R. C. A Conjugated Polymer Network Approach to Anticorrosion Coatings: Poly(Vinylcarbazole) Electrodeposition. *Ind. Eng. Chem. Res.* **2010**, *49* (20), 9789–9797. <https://doi.org/10.1021/ie100813t>.
- (90) Roitman, D. B.; Inaoka, S.; Advincula, R. C. Method for Depositing Electrically Conducting Polymer Films via Electrochemical Deposition of Precursor Polymers. US6533918B2, March 18, 2003. <https://patents.google.com/patent/US6533918B2/en> (accessed 2026-02-04).
- (91) Advincula, R. C.; Pernites, R. New Types of Electrodeposited Polymer Coatings with Reversible Wettability and Electro-Optical Properties. WO2012009238A2, January 19, 2012. <https://patents.google.com/patent/WO2012009238A2/en> (accessed 2026-02-04).
- (92) Roitman, D. B.; Inaoka, S.; Advincula, R. C. Method for Depositing Electrically Conducting Polymer Films via Electrochemical Deposition of Precursor Polymers.

- US6294245B1, September 25, 2001. <https://patents.google.com/patent/US6294245B1/en> (accessed 2026-02-04).
- (93) de Leon, A. C.; Imperial, R. E. S.; Chen, Q.; Advincula, R. C. One-Step Fabrication of Superhydrophobic/Superoleophilic Electrodeposited Polythiophene for Oil and Water Separation. *Macromol. Mater. Eng.* **2019**, *304* (7), 1800722. <https://doi.org/10.1002/mame.201800722>.
- (94) Pernites, R. B.; Ponnappati, R. R.; Advincula, R. C. Superhydrophobic–Superoleophilic Polythiophene Films with Tunable Wetting and Electrochromism. *Adv. Mater.* **2011**, *23* (28), 3207–3213. <https://doi.org/10.1002/adma.201100469>.
- (95) Foster, E. L.; Leon, A. C. C. D.; Mangadlao, J.; Advincula, R. Electropolymerized and Polymer Grafted Superhydrophobic, Superoleophilic, and Hemi-Wicking Coatings. *J. Mater. Chem.* **2012**, *22* (22), 11025–11031. <https://doi.org/10.1039/C2JM31067H>.
- (96) Foster, E. L.; Tria, M. C. R.; Pernites, R. B.; Addison, S. J.; Advincula, R. C. Patterned Polymer Brushes via Electrodeposited ATRP, ROMP, and RAFT Initiators on Colloidal Template Arrays. *Soft Matter* **2011**, *8* (2), 353–359. <https://doi.org/10.1039/C1SM06406A>.
- (97) Tiu, B. D. B.; Tiu, S. B.; Wen, A. M.; Lam, P.; Steinmetz, N. F.; Advincula, R. C. Free-Standing, Nanopatterned Janus Membranes of Conducting Polymer–Virus Nanoparticle Arrays. *Langmuir* **2016**, *32* (24), 6185–6193. <https://doi.org/10.1021/acs.langmuir.6b00808>.
- (98) Advincula, R. Methods for Preparing Polymer Coatings by Electrochemical Grafting of Polymer Brushes, Compositions Prepared Thereby and Compositions for Preparing the Coatings. US9079999B2, July 14, 2015. <https://patents.google.com/patent/US9079999B2/en> (accessed 2026-02-04).
- (99) Santos, C. M.; Mangadlao, J.; Ahmed, F.; Leon, A.; Advincula, R. C.; Rodrigues, D. F. Graphene Nanocomposite for Biomedical Applications: Fabrication, Antimicrobial and Cytotoxic Investigations. *Nanotechnology* **2012**, *23* (39), 395101. <https://doi.org/10.1088/0957-4484/23/39/395101>.
- (100) de Leon, A. C.; Rodier, B. J.; Luo, Q.; Hemmingsen, C. M.; Wei, P.; Abbasi, K.; Advincula, R.; Pentzer, E. B. Distinct Chemical and Physical Properties of Janus Nanosheets. *ACS Nano* **2017**, *11* (7), 7485–7493. <https://doi.org/10.1021/acsnano.7b04020>.
- (101) Caldoná, E. B.; de Leon, A. C. C.; Mangadlao, J. D.; Lim, K. J. A.; Pajarito, B. B.; Advincula, R. C. On the Enhanced Corrosion Resistance of Elastomer-Modified Polybenzoxazine/Graphene Oxide Nanocomposite Coatings. *React. Funct. Polym.* **2018**, *123*, 10–19. <https://doi.org/10.1016/j.reactfunctpolym.2017.12.004>.
- (102) Ramírez-Soria, E. H.; León-Silva, U.; Lara-Ceniceros, T. E.; Bazán-Díaz, L.; Advincula, R. C.; Bonilla-Cruz, J. Graphene Oxide Bifunctionalized with NH<sub>2</sub>/NH<sub>3</sub><sup>+</sup> and Their Outstanding-Performance against Corrosion. *Appl. Surf. Sci.* **2021**, *561*, 150048. <https://doi.org/10.1016/j.apsusc.2021.150048>.
- (103) Ramírez-Soria, E. H.; León-Silva, U.; Lara-Ceniceros, T. E.; Advincula, R. C.; Bonilla-Cruz, J. Reduced Graphene Oxide Nanoplatelets Functionalized with Nonpolar Aliphatic Groups for High-Performance Coatings against Corrosion. *ACS Appl. Nano Mater.* **2022**, *5* (11), 16760–16773. <https://doi.org/10.1021/acsanm.2c03758>.
- (104) Ramírez-Soria, E. H.; León-Silva, U.; Rejón-García, L.; Lara-Ceniceros, Tania. E.; Advincula, R. C.; Bonilla-Cruz, J. Super-Anticorrosive Materials Based on Bifunctionalized Reduced Graphene Oxide. *ACS Appl. Mater. Interfaces* **2020**, *12* (40), 45254–45265. <https://doi.org/10.1021/acsam.0c11004>.

- (105) Ramírez-Soria, E. H.; León-Silva, U.; Trejo-Maldonado, M.; Lara-Ceniceros, T. E.; Aguilar-Elguezabal, A.; Silva-Vidaurre, G.; Advincula, R. C.; Bonilla-Cruz, J. On the Use of Aromatic-Functionalized Reduced Graphene Oxide to Confine Corrosive Ions in Nanocomposite Coatings. *Prog. Org. Coat.* **2024**, *188*, 108263. <https://doi.org/10.1016/j.porgcoat.2024.108263>.
- (106) Mangadlao, J. D.; Cao, P.; Choi, D.; Advincula, R. C. Photoreduction of Graphene Oxide and Photochemical Synthesis of Graphene–Metal Nanoparticle Hybrids by Ketyl Radicals. *ACS Appl. Mater. Interfaces* **2017**, *9* (29), 24887–24898. <https://doi.org/10.1021/acsami.7b06275>.
- (107) Mangadlao, J. D.; Lim, K. J.; Danda, C.; Dalida, M. L.; Advincula, R. C. House of Cards Nanostructuring of Graphene Oxide and Montmorillonite Clay for Oil–Water Separation. *Macromol. Mater. Eng.* **2018**, *303* (1), 1700314. <https://doi.org/10.1002/mame.201700314>.
- (108) Buruga, K.; Song, H.; Shang, J.; Bolan, N.; Jagannathan, T. K.; Kim, K.-H. A Review on Functional Polymer-Clay Based Nanocomposite Membranes for Treatment of Water. *J. Hazard. Mater.* **2019**, *379*, 120584. <https://doi.org/10.1016/j.jhazmat.2019.04.067>.
- (109) Fan, X.; Xia, C.; Advincula, R. C. Intercalation of Polymerization Initiators into Montmorillonite Nanoparticle Platelets: Free Radical vs. Anionic Initiator Clays. *Colloids Surf. Physicochem. Eng. Asp.* **2003**, *219* (1), 75–86. [https://doi.org/10.1016/S0927-7757\(03\)00013-X](https://doi.org/10.1016/S0927-7757(03)00013-X).
- (110) Chen, Q.; Tang, Y.; Advincula, R. C. Superhydrophobic and Anti-Corrosion Properties in Thiol-Ene Graphene Oxide Nanocomposite Coatings. *MRS Commun.* **2023**, *13* (5), 917–925. <https://doi.org/10.1557/s43579-023-00460-0>.
- (111) Santos, C. M.; Tria, M. C. R.; Vergara, R. A. M. V.; Ahmed, F.; Advincula, R. C.; Rodrigues, D. F. Antimicrobial Graphene Polymer (PVK-GO) Nanocomposite Films. *Chem. Commun.* **2011**, *47* (31), 8892–8894. <https://doi.org/10.1039/C1CC11877C>.
- (112) Mejias Carpio, I. E.; Mangadlao, J. D.; Nguyen, H. N.; Advincula, R. C.; Rodrigues, D. F. Graphene Oxide Functionalized with Ethylenediamine Triacetic Acid for Heavy Metal Adsorption and Anti-Microbial Applications. *Carbon* **2014**, *77*, 289–301. <https://doi.org/10.1016/j.carbon.2014.05.032>.
- (113) Rodrigues, D. F.; Advincula, R. C.; Claydon, F.; Santos, C. M.; Tria, M. C. R. Nanocomposite Polymer-Carbon Based Nanomaterial Filters for the Simultaneous Removal of Bacteria and Heavy Metals. US8925736B2, January 6, 2015. <https://patents.google.com/patent/US8925736B2/en> (accessed 2026-02-04).
- (114) Grande, C. D.; Mangadlao, J.; Fan, J.; De Leon, A.; Delgado-Ospina, J.; Rojas, J. G.; Rodrigues, D. F.; Advincula, R. Chitosan Cross-Linked Graphene Oxide Nanocomposite Films with Antimicrobial Activity for Application in Food Industry. *Macromol. Symp.* **2017**, *374* (1), 1600114. <https://doi.org/10.1002/masy.201600114>.
- (115) Ramírez-Soria, E.-H.; Bonilla-Cruz, J.; Flores-Amaro, M. G.; García, V. J.; Lara-Ceniceros, T. E.; Longoria-Rodríguez, F. E.; Elizondo, P.; Advincula, R. C. On the Effect of Ultralow Loading of Microwave-Assisted Bifunctionalized Graphene Oxide in Stereolithographic 3D-Printed Nanocomposites. *ACS Appl. Mater. Interfaces* **2020**, *12* (43), 49061–49072. <https://doi.org/10.1021/acsami.0c13702>.
- (116) Kostenbauder, H. B.; Boxenbaum, H. G.; Deluca, P. P. Nylon as a Dialysis Membrane. *J. Pharm. Sci.* **1969**, *58* (6), 753–757. <https://doi.org/10.1002/jps.2600580624>.

- (117) Xu, F. J.; Zhao, J. P.; Kang, E. T.; Neoh, K. G.; Li, J. Functionalization of Nylon Membranes via Surface-Initiated Atom-Transfer Radical Polymerization. *Langmuir* **2007**, *23* (16), 8585–8592. <https://doi.org/10.1021/la7011342>.
- (118) Alemayehu, H. G.; Hailu, R. B.; Tadesse, P. Highly Stable Graphene Oxide/Nylon Membrane for Molecular Separation. *Nanotechnology* **2023**, *34* (30), 305703. <https://doi.org/10.1088/1361-6528/acd060>.
- (119) de Leon, A. C.; Rodier, B. J.; Bajamundi, C.; Espera, A. Jr.; Wei, P.; Kwon, J. G.; Williams, J.; Ilijasic, F.; Advincula, R. C.; Pentzer, E. Plastic Metal-Free Electric Motor by 3D Printing of Graphene-Polyamide Powder. *ACS Appl. Energy Mater.* **2018**, *1* (4), 1726–1733. <https://doi.org/10.1021/acsaem.8b00240>.
- (120) Espera Jr., A. H.; Valino, A. D.; Palaganas, J. O.; Souza, L.; Chen, Q.; Advincula, R. C. 3D Printing of a Robust Polyamide-12-Carbon Black Composite via Selective Laser Sintering: Thermal and Electrical Conductivity. *Macromol. Mater. Eng.* **2019**, *304* (4), 1800718. <https://doi.org/10.1002/mame.201800718>.
- (121) Santos, C. M.; Milagros Cui, K.; Ahmed, F.; Tria, M. C. R.; Vergara, R. A. M. V.; de Leon, A. C.; Advincula, R. C.; Rodrigues, D. F. Bactericidal and Anticorrosion Properties in PVK/MWNT Nanocomposite Coatings on Stainless Steel. *Macromol. Mater. Eng.* **2012**, *297* (8), 807–813. <https://doi.org/10.1002/mame.201100334>.
- (122) Ahmed, F.; Santos, C. M.; Mangadla, J.; Advincula, R.; Rodrigues, D. F. Antimicrobial PVK:SWNT Nanocomposite Coated Membrane for Water Purification: Performance and Toxicity Testing. *Water Res.* **2013**, *47* (12), 3966–3975. <https://doi.org/10.1016/j.watres.2012.10.055>.
- (123) Advincula, R. Polymer Nanocomposite Precursors with Carbon Nanotubes and/or Graphene and Related Thin Films and Patterning. US8932671B2, January 13, 2015. <https://patents.google.com/patent/US8932671B2/en> (accessed 2026-02-04).
- (124) Mumtaz, F.; Faraz, M.; Balakrishnan, H. K.; Nair, R.; Dumée, L. F. Stimuli-Responsive Membranes—Mechanisms, Materials and Future Directions. *Npj Clean Water* **2025**, *9* (1), 1. <https://doi.org/10.1038/s41545-025-00533-8>.
- (125) *Deed - Attribution-NonCommercial-NoDerivatives 4.0 International - Creative Commons*. <https://creativecommons.org/licenses/by-nc-nd/4.0/> (accessed 2025-03-19).
- (126) Wandera, D.; Wickramasinghe, S. R.; Husson, S. M. Stimuli-Responsive Membranes. *J. Membr. Sci.* **2010**, *357* (1), 6–35. <https://doi.org/10.1016/j.memsci.2010.03.046>.
- (127) Cao, P.-F.; Mangadla, J. D.; Advincula, R. C. Stimuli-Responsive Polymers and Their Potential Applications in Oil-Gas Industry. *Polym. Rev.* **2015**, *55* (4), 706–733. <https://doi.org/10.1080/15583724.2015.1040553>.
- (128) Osti, N. C.; Remy, R. A.; Ehrhardt, D. A.; Hensley, D. K.; Chen, J.; Mamontov, E.; Advincula, R.; Nguyen, N. A. Sustainable Shape Memory Elastomers with Reduced Melt Viscosity and Enhanced Stiffness. *ACS Appl. Polym. Mater.* **2025**, *7* (4), 2554–2566. <https://doi.org/10.1021/acsapm.4c03810>.
- (129) Advincula, P. A.; Leon, A. C. de; Rodier, B. J.; Kwon, J.; Advincula, R. C.; Pentzer, E. B. Accommodating Volume Change and Imparting Thermal Conductivity by Encapsulation of Phase Change Materials in Carbon Nanoparticles. *J. Mater. Chem. A* **2018**, *6* (6), 2461–2467. <https://doi.org/10.1039/C7TA09664J>.
- (130) Chen, Q.; Cao, P.-F.; Advincula, R. C. Mechanically Robust, Ultraelastic Hierarchical Foam with Tunable Properties via 3D Printing. *Adv. Funct. Mater.* **2018**, *28* (21), 1800631. <https://doi.org/10.1002/adfm.201800631>.

- (131) Chen, Q.; Han, L.; Ren, J.; Rong, L.; Cao, P.; Advincula, R. C. 4D Printing via an Unconventional Fused Deposition Modeling Route to High-Performance Thermosets. *ACS Appl. Mater. Interfaces* **2020**, *12* (44), 50052–50060. <https://doi.org/10.1021/acsami.0c13976>.
- (132) Durmaz, E. N.; Sahin, S.; Virga, E.; de Beer, S.; de Smet, L. C. P. M.; de Vos, W. M. Polyelectrolytes as Building Blocks for Next-Generation Membranes with Advanced Functionalities. *ACS Appl. Polym. Mater.* **2021**, *3* (9), 4347–4374. <https://doi.org/10.1021/acsapm.1c00654>.
- (133) Regenspurg, J. A.; Jonkers, W. A.; Junker, M. A.; Achterhuis, I.; te Brinke, E.; de Vos, W. M. Polyelectrolyte Multilayer Membranes: An Experimental Review. *Desalination* **2024**, *583*, 117693. <https://doi.org/10.1016/j.desal.2024.117693>.
- (134) Jonkers, W. A.; Precheur, M.; Andrade, J. R.; de Vos, W. M.; te Brinke, E. Highly Selective Polyelectrolyte Multilayer Membranes Through Hydrophobic Interactions. *ACS Appl. Mater. Interfaces* **2025**, *17* (14), 21725–21735. <https://doi.org/10.1021/acsami.4c20150>.
- (135) Christakopoulos, P.; Wang, H.; Bonnesen, P. V.; Keum, J. K.; Wang, Y.; Hong, K.; Lokitz, B. S.; Doucet, M.; Browning, J. F.; Advincula, R. C.; Kumar, R. Characterizing Hygroscopic Films of Polyzwitterions in Electric Fields Using Neutron and X-Ray Reflectometries: Electrostriction or Mass Loss? *ACS Appl. Mater. Interfaces* **2024**, *16* (36), 48307–48319. <https://doi.org/10.1021/acsami.4c09938>.
- (136) Keum, J. K.; Christakopoulos, P.; Liu, Z.; Li, T.; Chen, J.; Williams, A.; Hensley, D. K.; Hong, K.; Wang, Y.; Advincula, R.; Kumar, R. Chemical Specificity in Polyzwitterion-Polyelectrolyte Coacervates: Polycations vs Polyanions. *Eur. Polym. J.* **2024**, *215*, 113177. <https://doi.org/10.1016/j.eurpolymj.2024.113177>.
- (137) Liu, Z.; Keum, J. K.; Li, T.; Chen, J.; Hong, K.; Wang, Y.; Sumpter, B. G.; Advincula, R.; Kumar, R. Anti-Polyelectrolyte and Polyelectrolyte Effects on Conformations of Polyzwitterionic Chains in Dilute Aqueous Solutions. *PNAS Nexus* **2023**, *2* (7), pgad204. <https://doi.org/10.1093/pnasnexus/pgad204>.
- (138) Jin, S.; Shan, X.; Tian, J.; Li, Y.; Ding, H.; Advincula, R.; Tian, M.; Cao, P.-F. High-Entropy Gel Polymer Electrolyte for Wide-Temperature Operatable Li-Metal Batteries. *Adv. Funct. Mater.* **2025**, *35* (45), 2500440. <https://doi.org/10.1002/adfm.202500440>.
- (139) Park, M.-K.; Advincula, R. C. The Layer-by-Layer Assemblies of Polyelectrolytes and Nanomaterials as Films and Particle Coatings. In *Functional Polymer Films*; John Wiley & Sons, Ltd, 2011; pp 73–112. <https://doi.org/10.1002/9783527638482.ch3>.
- (140) Park, M.-K.; Deng, S.; Advincula, R. C. pH-Sensitive Bipolar Ion-Permselective Ultrathin Films. *J. Am. Chem. Soc.* **2004**, *126* (42), 13723–13731. <https://doi.org/10.1021/ja0484707>.
- (141) Dante, S.; Advincula, R.; Frank, C. W.; Stroeve, P. Photoisomerization of Polyionic Layer-by-Layer Films Containing Azobenzene. *Langmuir* **1999**, *15* (1), 193–201. <https://doi.org/10.1021/la980497e>.
- (142) Kato, K.; Watanabe, N.; Katagiri, S.; Shinbo, K.; Kaneko, F.; Locklin, J.; Baba, A.; Advincula, R. C. Electrical Properties and Gas Response in Alternate Layer-by-Layer Films of Copper Phthalocyanine Dyes. *Jpn. J. Appl. Phys.* **2004**, *43* (4S), 2311. <https://doi.org/10.1143/JJAP.43.2311>.

- (143) Tiu, B. D. B.; Kernan, D. L.; Tiu, S. B.; Wen, A. M.; Zheng, Y.; Pokorski, J. K.; Advincula, R. C.; Steinmetz, N. F. Electrostatic Layer-by-Layer Construction of Fibrous TMV Biofilms. *Nanoscale* **2017**, *9* (4), 1580–1590. <https://doi.org/10.1039/C6NR06266K>.
- (144) Estillore, N. C.; Advincula, R. C. Stimuli-Responsive Binary Mixed Polymer Brushes and Free-Standing Films by LbL-SIP. *Langmuir* **2011**, *27* (10), 5997–6008. <https://doi.org/10.1021/la200089x>.
- (145) Estillore, N. C.; Advincula, R. C. Free-Standing Films of Semifluorinated Block Copolymer Brushes from Layer-by-Layer Polyelectrolyte Macroinitiators. *Macromol. Chem. Phys.* **2011**, *212* (15), 1552–1566. <https://doi.org/10.1002/macp.201100066>.
- (146) Fulghum, T. M.; Estillore, N. C.; Vo, C.-D.; Armes, S. P.; Advincula, R. C. Stimuli-Responsive Polymer Ultrathin Films with a Binary Architecture: Combined Layer-by-Layer Polyelectrolyte and Surface-Initiated Polymerization Approach. *Macromolecules* **2008**, *41* (2), 429–435. <https://doi.org/10.1021/ma0717136>.
- (147) de Leon, A.; Advincula, R. C. Reversible Superhydrophilicity and Superhydrophobicity on a Lotus-Leaf Pattern. *ACS Appl. Mater. Interfaces* **2014**, *6* (24), 22666–22672. <https://doi.org/10.1021/am506050k>.
- (148) Caruso, F.; Möhwald, H. Preparation and Characterization of Ordered Nanoparticle and Polymer Composite Multilayers on Colloids. *Langmuir* **1999**, *15* (23), 8276–8281. <https://doi.org/10.1021/la990426v>.
- (149) Caruso, F.; Schöler, C.; Kurth, D. G. Core–Shell Particles and Hollow Shells Containing Metallo-Supramolecular Components. *Chem. Mater.* **1999**, *11* (11), 3394–3399. <https://doi.org/10.1021/cm9911058>.
- (150) Sukhorukov, G. B.; Susha, A. S.; Davis, S.; Leporatti, S.; Donath, E.; Hartmann, J.; Möhwald, H. Precipitation of Inorganic Salts inside Hollow Micrometer-Sized Polyelectrolyte Shells. *J. Colloid Interface Sci.* **2002**, *247* (1), 251–254. <https://doi.org/10.1006/jcis.2001.8102>.
- (151) Yuan, Q.; Cayre, O. J.; Fujii, S.; Armes, S. P.; Williams, R. A.; Biggs, S. Responsive Core–Shell Latex Particles as Colloidosome Microcapsule Membranes. *Langmuir* **2010**, *26* (23), 18408–18414. <https://doi.org/10.1021/la1033564>.
- (152) Donath, E.; Moya, S.; Neu, B.; Sukhorukov, G. B.; Georgieva, R.; Voigt, A.; Bäuml, H.; Kiesewetter, H.; Möhwald, H. Hollow Polymer Shells from Biological Templates: Fabrication and Potential Applications. *Chem. – Eur. J.* **2002**, *8* (23), 5481–5485. [https://doi.org/10.1002/1521-3765\(20021202\)8:23%3C5481::AID-CHEM5481%3E3.0.CO;2-8](https://doi.org/10.1002/1521-3765(20021202)8:23%3C5481::AID-CHEM5481%3E3.0.CO;2-8).
- (153) Park, M.-K.; Deng, S.; Advincula, R. C. Sustained Release Control via Photo-Cross-Linking of Polyelectrolyte Layer-by-Layer Hollow Capsules. *Langmuir* **2005**, *21* (12), 5272–5277. <https://doi.org/10.1021/la047008x>.
- (154) Park, M.-K.; Onishi, K.; Locklin, J.; Caruso, F.; Advincula, R. C. Self-Assembly and Characterization of Polyaniline and Sulfonated Polystyrene Multilayer-Coated Colloidal Particles and Hollow Shells. *Langmuir* **2003**, *19* (20), 8550–8554. <https://doi.org/10.1021/la034827t>.
- (155) Fulghum, T. M.; Patton, D. L.; Advincula, R. C. Fuzzy Ternary Particle Systems by Surface-Initiated Atom Transfer Radical Polymerization from Layer-by-Layer Colloidal Core–Shell Macroinitiator Particles. *Langmuir* **2006**, *22* (20), 8397–8402. <https://doi.org/10.1021/la0601509>.

- (156) Partridge, A. C.; Milestone, C.; Too, C. O.; Wallace, G. G. Ion Transport Membranes Based on Conducting Polymers. *J. Membr. Sci.* **1997**, *132* (2), 245–253. [https://doi.org/10.1016/S0376-7388\(97\)00072-0](https://doi.org/10.1016/S0376-7388(97)00072-0).
- (157) Price, W. E.; Too, C. O.; Wallace, G. G.; Zhou, D. Development of Membrane Systems Based on Conducting Polymers. *Synth. Met.* **1999**, *102* (1), 1338–1341. [https://doi.org/10.1016/S0379-6779\(98\)90212-0](https://doi.org/10.1016/S0379-6779(98)90212-0).
- (158) Escorihuela, J.; Narducci, R.; Compañ, V.; Costantino, F. Proton Conductivity of Composite Polyelectrolyte Membranes with Metal–Organic Frameworks for Fuel Cell Applications. *Adv. Mater. Interfaces* **2019**, *6* (2), 1801146. <https://doi.org/10.1002/admi.201801146>.
- (159) Waenkaew, P.; Phanichphant, S.; Advincula, R. C. Electropolymerization of Layer-by-Layer Precursor Polymer Films. *Polym. Adv. Technol.* **2011**, *22* (5), 753–758. <https://doi.org/10.1002/pat.1886>.
- (160) Huang, C.; Jiang, G.; Advincula, R. Electrochemical Cross-Linking and Patterning of Nanostructured Polyelectrolyte–Carbazole Precursor Ultrathin Films. *Macromolecules* **2008**, *41* (13), 4661–4670. <https://doi.org/10.1021/ma800268n>.
- (161) Armstrong, S. R.; Du, J.; Baer, E. Co-Extruded Multilayer Shape Memory Materials: Nano-Scale Phenomena. *Polymer* **2014**, *55* (2), 626–631. <https://doi.org/10.1016/j.polymer.2013.11.044>.
- (162) Wu, H.; Zhang, J.; Zhang, C.; Feng, J.; Rahman, Md. A.; Baer, E. Structure–Properties Relationship of a Novel Multilayer Film/Foam Material Produced through Co-Extrusion and Orientation. *Ind. Eng. Chem. Res.* **2016**, *55* (41), 10947–10954. <https://doi.org/10.1021/acs.iecr.6b03418>.
- (163) Wang, X.; Price, E. J.; Wnek, G. E.; Olah, A.; Baer, E. Oriented Tapes of Incompatible Polymers Using a Novel Multiplication Co-Extrusion Process. *Polymers* **2022**, *14* (18), 3872. <https://doi.org/10.3390/polym14183872>.
- (164) Armstrong, S. R.; Offord, G. T.; Paul, D. R.; Freeman, B. D.; Hiltner, A.; Baer, E. Co-Extruded Polymeric Films for Gas Separation Membranes. *J. Appl. Polym. Sci.* **2014**, *131* (2). <https://doi.org/10.1002/app.39765>.
- (165) Feng, J.; Zhang, G.; MacInnis, K.; Olah, A.; Baer, E. Structure-Property Relationships of Microporous Membranes Produced by Biaxial Orientation of Compatibilized PP/Nylon 6 Blends. *Polymer* **2018**, *145*, 148–156. <https://doi.org/10.1016/j.polymer.2018.05.005>.
- (166) Advincula, R.; Chao, P.; Baer, E. Multilayer Polymer Composite Constructs. US11364656B2, June 21, 2022. <https://patents.google.com/patent/US11364656B2/en> (accessed 2026-02-04).
- (167) LEON, A. de; Advincula, R. C.; Baer, E. Multilayered Anisotropic Microparticles. US20200122378A1, April 23, 2020. <https://patents.google.com/patent/US20200122378A1/en> (accessed 2026-02-24).
- (168) Tiu, B. D. B.; Nguyen, H. N.; Rodrigues, D. F.; Advincula, R. C. Electrospinning Superhydrophobic and Antibacterial PS/MWNT Nanofibers onto Multilayer Gas Barrier Films. *Macromol. Symp.* **2017**, *374* (1), 1600138. <https://doi.org/10.1002/masy.201600138>.
- (169) Pangilinan, K. D.; de Leon, A. C. C.; Mangadlao, J. D.; Baer, E.; Advincula, R. C. Grafting of a Stimuli Responsive Polymer on Nanolayered Coextruded PS/PCL Films by Surface Initiated Polymerization. *Macromol. Mater. Eng.* **2016**, *301* (7), 870–875. <https://doi.org/10.1002/mame.201600019>.

- (170) Cimatu, K. L. A.; Ambagaspitiya, T. D.; Premadasa, U. I.; Adhikari, N. M.; Kruse, A.; Robertson, E.; Guan, S.; Rong, L.; Advincula, R.; Bythell, B. J. Polymer-Solvent Interaction and Conformational Changes at a Molecular Level: Implication to Solvent-Assisted Deformation and Aggregation at the Polymer Surface. *J. Colloid Interface Sci.* **2022**, *616*, 221–233. <https://doi.org/10.1016/j.jcis.2022.02.006>.
- (171) Schweidtmann, A. M.; Esche, E.; Fischer, A.; Kloft, M.; Repke, J.-U.; Sager, S.; Mitsos, A. Machine Learning in Chemical Engineering: A Perspective. *Chem. Ing. Tech.* **2021**, *93* (12), 2029–2039. <https://doi.org/10.1002/cite.202100083>.
- (172) Badillo, S.; Banfai, B.; Birzele, F.; Davydov, I. I.; Hutchinson, L.; Kam-Thong, T.; Siebourg-Polster, J.; Steiert, B.; Zhang, J. D. An Introduction to Machine Learning. *Clin. Pharmacol. Ther.* **2020**, *107* (4), 871–885. <https://doi.org/10.1002/cpt.1796>.
- (173) Choudhary, K.; Kelley, M. L. ChemNLP: A Natural Language-Processing-Based Library for Materials Chemistry Text Data. *J. Phys. Chem. C* **2023**, *127* (35), 17545–17555. <https://doi.org/10.1021/acs.jpcc.3c03106>.
- (174) Karanikolas, N. N.; Manga, E.; Samaridi, N.; Stergiopoulos, V.; Tousidou, E.; Vassilakopoulos, M. Strengths and Weaknesses of LLM-Based and Rule-Based NLP Technologies and Their Potential Synergies. *Electronics* **2025**, *14* (15), 3064. <https://doi.org/10.3390/electronics14153064>.
- (175) Xiao, Y.; Liu, J.; Zheng, Y.; Xie, X.; Hao, J.; Li, M.; Wang, R.; Ni, F.; Li, Y.; Luo, J.; Jiao, S.; Peng, J. CellAgent: An LLM-Driven Multi-Agent Framework for Automated Single-Cell Data Analysis. arXiv July 13, 2024. <https://doi.org/10.48550/arXiv.2407.09811>.
- (176) Inizan, T. J.; Yang, S.; Kaplan, A.; Lin, Y.; Yin, J.; Mirzaei, S.; Abdelgaid, M.; Alawadhi, A. H.; Cho, K.; Zheng, Z.; Cubuk, E. D.; Borgs, C.; Chayes, J. T.; Persson, K. A.; Yaghi, O. M. System of Agentic AI for the Discovery of Metal-Organic Frameworks. arXiv April 18, 2025. <https://doi.org/10.48550/arXiv.2504.14110>.
- (177) Ansari, M.; Mohamad Moosavi, S. Agent-Based Learning of Materials Datasets from the Scientific Literature. *Digit. Discov.* **2024**, *3* (12), 2607–2617. <https://doi.org/10.1039/D4DD000252K>.
- (178) Gridach, M.; Nanavati, J.; Abidine, K. Z. E.; Mendes, L.; Mack, C. Agentic AI for Scientific Discovery: A Survey of Progress, Challenges, and Future Directions. arXiv March 12, 2025. <https://doi.org/10.48550/arXiv.2503.08979>.
- (179) Chen, K.; Lu, J.; Li, J.; Yang, X.; Du, Y.; Wang, K.; Shi, Q.; Yu, J.; Li, L.; Qiu, J.; Pan, J.; Huang, Y.; Fang, Q.; Heng, P. A.; Chen, G. *Chemist-X: Large Language Model-empowered Agent for Reaction Condition Recommendation in Chemical Synthesis*. arXiv.org. <https://arxiv.org/abs/2311.10776v6> (accessed 2026-01-08).
- (180) Tian, W.; Gong, L.; Yu, C.; Zhou, Y. A Molecular Dynamics Simulation Study on Hydrocarbon Ladder Polymer Membranes for Gas Separation. *Phys. Chem. Chem. Phys.* **2025**, *27* (11), 5832–5842. <https://doi.org/10.1039/D4CP04588B>.
- (181) Ortiz-Albo, P.; Takaba, H.; Kumakiri, I.; Crespo, J. G.; Neves, L. A. An Overview of Molecular Simulations Studies in Mixed Matrix Membranes for Gas Separation Processes. *J. Membr. Sci. Res.* **2022**, *8* (4), e253969. <https://doi.org/10.22079/jmsr.2022.549436.1536>.
- (182) Liu, Y.; Li, N.; Cui, X.; Yan, W.; Su, J.; Jin, L. A Review on the Morphology and Material Properties of the Gas Separation Membrane: Molecular Simulation. *Membranes* **2022**, *12* (12), 1274. <https://doi.org/10.3390/membranes12121274>.
- (183) Daglar, H.; Keskin, S. Combining Machine Learning and Molecular Simulations to Unlock Gas Separation Potentials of MOF Membranes and MOF/Polymer MMMs. *ACS*

- Appl. Mater. Interfaces* **2022**, *14* (28), 32134–32148.  
<https://doi.org/10.1021/acsami.2c08977>.
- (184) Da Conceicao, M.; Nemetz, L.; Rivero, J.; Hornbostel, K.; Lipscomb, G. Gas Separation Membrane Module Modeling: A Comprehensive Review. *Membranes* **2023**, *13* (7), 639.  
<https://doi.org/10.3390/membranes13070639>.
- (185) Giro, R.; Hsu, H.; Kishimoto, A.; Hama, T.; Neumann, R. F.; Luan, B.; Takeda, S.; Hamada, L.; Steiner, M. B. AI Powered, Automated Discovery of Polymer Membranes for Carbon Capture. *Npj Comput. Mater.* **2023**, *9* (1), 133.  
<https://doi.org/10.1038/s41524-023-01088-3>.
- (186) Basdogan, Y.; Pollard, D. R.; Shastry, T.; Carbone, M. R.; Kumar, S. K.; Wang, Z.-G. Machine Learning-Guided Discovery of Polymer Membranes for CO<sub>2</sub> Separation with Genetic Algorithm. *J. Membr. Sci.* **2024**, *712*, 123169. <https://doi.org/10.1016/j.memsci.2024.123169>.
- (187) Talukder, M. J.; Alshami, A. S.; Tayyebi, A.; Ismail, N.; Yu, X. Membrane Science Meets Machine Learning: Future and Potential Use in Assisting Membrane Material Design and Fabrication. *Sep. Purif. Rev.* **2024**, *53* (2), 216–229.  
<https://doi.org/10.1080/15422119.2023.2212295>.
- (188) Yogarathinam, L. T.; Abba, S. I.; Usman, J.; Ramamoorthy, M.; Aljundi, I. H. Interpretable SHAP-Based Machine Learning-Assisted Design for Selecting Ultrafiltration Membranes in Protein-Laden Phosphate Wastewater. *Clean. Chem. Eng.* **2025**, *11*, 100187.  
<https://doi.org/10.1016/j.clce.2025.100187>.
- (189) Scheichl, R.; Klopffer, M.-H.; Benjelloun-Dabaghi, Z.; Flaconnèche, B. Permeation of Gases in Polymers: Parameter Identification and Nonlinear Regression Analysis. *J. Membr. Sci.* **2005**, *254* (1), 275–293. <https://doi.org/10.1016/j.memsci.2005.01.019>.
- (190) Maleki, R.; Shams, S. M.; Chellehbari, Y. M.; Rezvantalab, S.; Jahromi, A. M.; Asadnia, M.; Abbassi, R.; Aminabhavi, T.; Razmjou, A. Materials Discovery of Ion-Selective Membranes Using Artificial Intelligence. *Commun. Chem.* **2022**, *5* (1), 132.  
<https://doi.org/10.1038/s42004-022-00744-x>.
- (191) Glass, S.; Schmidt, M.; Merten, P.; Abdul Latif, A.; Fischer, K.; Schulze, A.; Friederich, P.; Filiz, V. Design of Modified Polymer Membranes Using Machine Learning. *ACS Appl. Mater. Interfaces* **2024**, *16* (16), 20990–21000. <https://doi.org/10.1021/acsami.3c18805>.
- (192) Cao, Z.; Barati Farimani, O.; Ock, J.; Barati Farimani, A. Machine Learning in Membrane Design: From Property Prediction to AI-Guided Optimization. *Nano Lett.* **2024**, *24* (10), 2953–2960. <https://doi.org/10.1021/acs.nanolett.3c05137>.
- (193) Jeong, N.; Epsztein, R.; Wang, R.; Park, S.; Lin, S.; Tong, T. Exploring the Knowledge Attained by Machine Learning on Ion Transport across Polyamide Membranes Using Explainable Artificial Intelligence. *Environ. Sci. Technol.* **2023**, *57* (46), 17851–17862.  
<https://doi.org/10.1021/acs.est.2c08384>.
- (194) Cairone, S.; Hasan, S. W.; Choo, K.-H.; Li, C.-W.; Zarra, T.; Belgiorno, V.; Naddeo, V. Integrating Artificial Intelligence Modeling and Membrane Technologies for Advanced Wastewater Treatment: Research Progress and Future Perspectives. *Sci. Total Environ.* **2024**, *944*, 173999. <https://doi.org/10.1016/j.scitotenv.2024.173999>.
- (195) Nazari, S.; Abdelrasoul, A. Advancements and Applications of Artificial Intelligence and Machine Learning in Material Science and Membrane Technology: A Comprehensive Review. *Membranes* **2025**, *15* (12), 353. <https://doi.org/10.3390/membranes15120353>.

- (196) Hameed, M. U.; Amjad, Z.; Al Alwan, B.; El Jery, A.; Hassan, H. M. A.; Ali, L.; Ahmad, A.; Khan, S.; Raza, S. Recent Progress in 2D-MXene-Based Membranes for Water Treatments; Fabrication, Properties, and Advanced Desalination Application. *Desalination* **2025**, *599*, 118462. <https://doi.org/10.1016/j.desal.2024.118462>.
- (197) Guan, H.; Wang, M.; Huang, X.; Dong, Y.; Liu, J. An Artificial Intelligence Framework for Separation Performance Prediction of Polymeric Pervaporation Membranes. *Desalination* **2026**, *617*, 119423. <https://doi.org/10.1016/j.desal.2025.119423>.
- (198) Shahouni, R.; Abbasi, M.; Dibaj, M.; Akrami, M. Utilising Artificial Intelligence to Predict Membrane Behaviour in Water Purification and Desalination. *Water* **2024**, *16* (20), 2940. <https://doi.org/10.3390/w16202940>.
- (199) Barnett, J. W.; Bilchak, C. R.; Wang, Y.; Benicewicz, B. C.; Murdock, L. A.; Bereau, T.; Kumar, S. K. Designing Exceptional Gas-Separation Polymer Membranes Using Machine Learning. *Sci. Adv.* **2020**, *6* (20), eaaz4301. <https://doi.org/10.1126/sciadv.aaz4301>.
- (200) Tijing, L. D.; Dizon, J. R. C.; Ibrahim, I.; Nisay, A. R. N.; Shon, H. K.; Advincula, R. C. 3D Printing for Membrane Separation, Desalination and Water Treatment. *Appl. Mater. Today* **2020**, *18*, 100486. <https://doi.org/10.1016/j.apmt.2019.100486>.
- (201) Caldon, E. B.; Dizon, J. R. C.; Espera, A. H. Jr.; Advincula, R. C. On the Economic, Environmental, and Sustainability Aspects of 3D Printing toward a Cyclic Economy. In *Energy Transition: Climate Action and Circularity*; ACS Symposium Series; American Chemical Society, 2022; Vol. 1412, pp 507–525. <https://doi.org/10.1021/bk-2022-1412.ch011>.
- (202) Valino, A. D.; Dizon, J. R. C.; Espera, A. H.; Chen, Q.; Messman, J.; Advincula, R. C. Advances in 3D Printing of Thermoplastic Polymer Composites and Nanocomposites. *Prog. Polym. Sci.* **2019**, *98*, 101162. <https://doi.org/10.1016/j.progpolymsci.2019.101162>.
- (203) Jiang, Y.; Serrano, A. X.; Choi, W.; Advincula, R. C.; Wu, H. F. Advanced and Functional Composite Materials via Additive Manufacturing: Trends and Perspectives. *MRS Commun.* **2024**, *14* (4), 449–459. <https://doi.org/10.1557/s43579-024-00625-5>.
- (204) de Leon, A. C.; Chen, Q.; Palaganas, N. B.; Palaganas, J. O.; Manapat, J.; Advincula, R. C. High Performance Polymer Nanocomposites for Additive Manufacturing Applications. *React. Funct. Polym.* **2016**, *103*, 141–155. <https://doi.org/10.1016/j.reactfunctpolym.2016.04.010>.
- (205) Harding, M. J.; Brady, S.; O'Connor, H.; Lopez-Rodriguez, R.; Edwards, M. D.; Tracy, S.; Dowling, D.; Gibson, G.; Girard, K. P.; Ferguson, S. 3D Printing of PEEK Reactors for Flow Chemistry and Continuous Chemical Processing. *React. Chem. Eng.* **2020**, *5* (4), 728–735. <https://doi.org/10.1039/C9RE00408D>.
- (206) Bao, Y. Recent Trends in Advanced Photoinitiators for Vat Photopolymerization 3D Printing. *Macromol. Rapid Commun.* **2022**, *43* (14), 2200202. <https://doi.org/10.1002/marc.202200202>.
- (207) Chekkaramkodi, D.; Jacob, L.; C, M. S.; Umer, R.; Butt, H. Review of Vat Photopolymerization 3D Printing of Photonic Devices. *Addit. Manuf.* **2024**, *86*, 104189. <https://doi.org/10.1016/j.addma.2024.104189>.
- (208) Martinez, A. C.; Schiaffino, E. M.; Aranzola, A. P.; Fernandez, C. A.; Seol, M.-L.; Sherrard, C. G.; Jones, J.; Huddleston, W. H.; Dornbusch, D. A.; Sreenivasan, S. T.; Cortes, P.; MacDonald, E.; Maurel, A. Multiprocess 3D Printing of Sodium-Ion Batteries via Vat Photopolymerization and Direct Ink Writing. *J. Phys. Energy* **2023**, *5* (4), 045010. <https://doi.org/10.1088/2515-7655/acf958>.

- (209) Thiam, B. G.; El Magri, A.; Vanaei, H. R.; Vaudreuil, S. 3D Printed and Conventional Membranes—A Review. *Polymers* **2022**, *14* (5), 1023. <https://doi.org/10.3390/polym14051023>.
- (210) Qian, X.; Ostwal, M.; Asatekin, A.; Geise, G. M.; Smith, Z. P.; Phillip, W. A.; Lively, R. P.; McCutcheon, J. R. A Critical Review and Commentary on Recent Progress of Additive Manufacturing and Its Impact on Membrane Technology. *J. Membr. Sci.* **2022**, *645*, 120041. <https://doi.org/10.1016/j.memsci.2021.120041>.
- (211) Roy Barman, S.; Gavit, P.; Chowdhury, S.; Chatterjee, K.; Nain, A. 3D-Printed Materials for Wastewater Treatment. *JACS Au* **2023**, *3* (11), 2930–2947. <https://doi.org/10.1021/jacsau.3c00409>.
- (212) Zhang, J.; Li, Y.; He, B.; Zhang, T.; Yang, B.; Yu, W.; Hu, L.; Jiang, G. 3D-Printed Flexible Thermoplastic Polyurethane Membrane for Ultrafast Oil/Water Separation. *Chem. Eng. J.* **2025**, *503*, 158500. <https://doi.org/10.1016/j.cej.2024.158500>.
- (213) Wei, P.; Leng, H.; Chen, Q.; Advincula, R. C.; Pentzer, E. B. Reprocessable 3D-Printed Conductive Elastomeric Composite Foams for Strain and Gas Sensing. *ACS Appl. Polym. Mater.* **2019**, *1* (4), 885–892. <https://doi.org/10.1021/acsapm.9b00118>.
- (214) Chen, Q.; Zhao, J.; Ren, J.; Rong, L.; Cao, P.-F.; Advincula, R. C. 3D Printed Multifunctional, Hyperelastic Silicone Rubber Foam. *Adv. Funct. Mater.* **2019**, *29* (23), 1900469. <https://doi.org/10.1002/adfm.201900469>.
- (215) Garcia, V. J.; Fazley Elahee, G. M.; Collera, A. K.; Thornton, T.; Cheng, X.; Rohan, S.; Howard, E. L.; Espera, A. H.; Advincula, R. C. On the Direct Ink Write (DIW) 3D Printing of Styrene-Butadiene Rubber (SBR)-Based Adhesive Sealant. *MRS Commun.* **2023**, *13* (6), 1266–1274. <https://doi.org/10.1557/s43579-023-00436-0>.
- (216) Nocheseda, C. J. C.; Fazley Elahee, G. M.; Santos, M. F. A.; Cheng, X.; Espera, A. H.; Advincula, R. C. On the 3D Printability of One-Part Moisture-Curable Polyurethanes via Direct Ink Writing (DIW). *MRS Commun.* **2023**, *13* (4), 647–656. <https://doi.org/10.1557/s43579-023-00407-5>.
- (217) Moczadlo, M.; Chen, Q.; Cheng, X.; Smith, Z. J.; Caldon, E. B.; Advincula, R. C. On the 3D Printing of Polypropylene and Post-Processing Optimization of Thermomechanical Properties. *MRS Commun.* **2023**, *13* (1), 169–176. <https://doi.org/10.1557/s43579-023-00329-2>.
- (218) Tai, S. L.; Abidin, M. N. Z.; Ma'amor, A.; Hashim, N. A.; Hashim, M. L. H. Polyethylene Terephthalate Membrane: A Review of Fabrication Techniques, Separation Processes, and Modifications. *Sep. Purif. Technol.* **2025**, *354*, 129343. <https://doi.org/10.1016/j.seppur.2024.129343>.
- (219) Shu, H.; Wang, C.; Yang, L.; Sun, D.; Song, C.; Zhang, X.; Chen, D.; Ma, Y.; Yang, W. Preparation of Multifunctional PET Membrane and Its Application in High-Efficiency Filtration and Separation in Complex Environment. *J. Hazard. Mater.* **2024**, *474*, 134669. <https://doi.org/10.1016/j.jhazmat.2024.134669>.
- (220) Holcomb, G.; Caldon, E. B.; Cheng, X.; Advincula, R. C. On the Optimized 3D Printing and Post-Processing of PETG Materials. *MRS Commun.* **2022**, *12* (3), 381–387. <https://doi.org/10.1557/s43579-022-00188-3>.
- (221) Siacor, F. D. C.; Chen, Q.; Zhao, J. Y.; Han, L.; Valino, A. D.; Taboada, E. B.; Caldon, E. B.; Advincula, R. C. On the Additive Manufacturing (3D Printing) of Viscoelastic Materials and Flow Behavior: From Composites to Food Manufacturing. *Addit. Manuf.* **2021**, *45*, 102043. <https://doi.org/10.1016/j.addma.2021.102043>.

- (222) Yazdi, M. K.; Vatanpour, V.; Taghizadeh, A.; Taghizadeh, M.; Ganjali, M. R.; Munir, M. T.; Habibzadeh, S.; Saeb, M. R.; Ghaedi, M. Hydrogel Membranes: A Review. *Mater. Sci. Eng. C* **2020**, *114*, 111023. <https://doi.org/10.1016/j.msec.2020.111023>.
- (223) Abdel-Rahman, R. M.; Abdel-Mohsen, A. M.; Frankova, J.; Piana, F.; Kalina, L.; Gajdosova, V.; Kapralkova, L.; Thottappali, M. A.; Jancar, J. Self-Assembled Hydrogel Membranes with Structurally Tunable Mechanical and Biological Properties. *Biomacromolecules* **2024**, *25* (6), 3449–3463. <https://doi.org/10.1021/acs.biomac.4c00082>.
- (224) Dizon, J. R. C.; Chen, Q.; Valino, A. D.; Advincula, R. C. Thermo-Mechanical and Swelling Properties of Three-Dimensional-Printed Poly (Ethylene Glycol) Diacrylate/Silica Nanocomposites. *MRS Commun.* **2019**, *9* (1), 209–217. <https://doi.org/10.1557/mrc.2018.188>.
- (225) Caldon, E. B.; Dizon, J. R. C.; Viers, R. A.; Garcia, V. J.; Smith, Z. J.; Advincula, R. C. Additively Manufactured High-Performance Polymeric Materials and Their Potential Use in the Oil and Gas Industry. *MRS Commun.* **2021**, *11* (6), 701–715. <https://doi.org/10.1557/s43579-021-00134-9>.
- (226) Aristizábal, S. L.; Chisca, S.; Pulido, B. A.; Nunes, S. P. Preparation of PEEK Membranes with Excellent Stability Using Common Organic Solvents. *Ind. Eng. Chem. Res.* **2020**, *59* (12), 5218–5226. <https://doi.org/10.1021/acs.iecr.9b04281>.
- (227) Wang, R.; Cheng, K.; Advincula, R. C.; Chen, Q. On the Thermal Processing and Mechanical Properties of 3D-Printed Polyether Ether Ketone. *MRS Commun.* **2019**, *9* (3), 1046–1052. <https://doi.org/10.1557/mrc.2019.86>.
- (228) Emolaga, C. S.; Arañez, S. A. C.; Yro, P. A. N. D.; Reyes, J. P.; Visaya, B. A.; Basilia, B. A.; Advincula, R. C. Surface Design of 3D-Printed PEEK by Controlling Slicing Parameters. *Int. J. Mech. Eng. Robot. Res.* **2022**, 181–186. <https://doi.org/10.18178/ijmerr.11.3.181-186>.
- (229) Emolaga, C. S.; Yro, P. A. N. D.; Aranez, S. A. C.; Reyes, J. P.; Visaya, B. A.; Basilia, B. A.; Monsada, A. M.; Advincula, R. Void Content Measurement of the 3D Printed PEEK Materials by X-Ray Micro Computed Tomography. *Diffus. Found. Mater. Appl.* **2022**, *31*, 29–35. <https://doi.org/10.4028/p-c00t77>.
- (230) Gao, Y.; Zhou, X.; Zhang, M.; Lyu, L.; Li, Z. Polyphenylene Sulfide-Based Membranes: Recent Progress and Future Perspectives. *Membranes* **2022**, *12* (10), 924. <https://doi.org/10.3390/membranes12100924>.
- (231) Foong, Y. X.; Yew, L. H.; Chai, P. V. Green Approaches to Polysulfone Based Membrane Preparation via Dimethyl Sulfoxide and Eco-Friendly Natural Additive Gum Arabic. *Mater. Today Proc.* **2021**, *46*, 2092–2097. <https://doi.org/10.1016/j.matpr.2021.04.470>.
- (232) Yang, C.; Han, N.; Wang, W.; Zhang, W.; Han, C.; Cui, Z.; Zhang, X. Fabrication of a PPS Microporous Membrane for Efficient Water-in-Oil Emulsion Separation. *Langmuir* **2018**, *34* (36), 10580–10590. <https://doi.org/10.1021/acs.langmuir.8b02393>.
- (233) Smith, Z. J.; Golias, C. J.; Vaske, T. J.; Young, S. A.; Chen, Q.; Goodbred, L.; Rong, L.; Cheng, X.; Penumadu, D.; Advincula, R. C. Correlating Viscosity and Die Swell in 3D Printing of Polyphenylsulfone: A Thermo-Mechanical Optimization Modus Operandi. *React. Funct. Polym.* **2024**, *194*, 105795. <https://doi.org/10.1016/j.reactfunctpolym.2023.105795>.
- (234) Soufyani, M.; Jei, T.; Bourret, D.; Sivade, A.; Larbot, A. Silicone Modified Silica Membrane. Application to the Gas Separation. *Sep. Purif. Technol.* **2001**, *25* (1), 451–457. [https://doi.org/10.1016/S1383-5866\(01\)00074-0](https://doi.org/10.1016/S1383-5866(01)00074-0).

- (235) Jha, P.; Mason, L. W.; Douglas Way, J. Characterization of Silicone Rubber Membrane Materials at Low Temperature and Low Pressure Conditions. *J. Membr. Sci.* **2006**, *272* (1), 125–136. <https://doi.org/10.1016/j.memsci.2005.07.039>.
- (236) Jiang, X.; Kumar, A. Performance of Silicone-Coated Polymeric Membrane in Separation of Hydrocarbons and Nitrogen Mixtures. *J. Membr. Sci.* **2005**, *254* (1), 179–188. <https://doi.org/10.1016/j.memsci.2004.12.041>.
- (237) Pan, L.-Q.; Zheng, Q.-N.; Feng, Q.-H.; Shen, Y.-B.; Hu, W.-Y.; Cao, C.-F.; Zhang, G.-D.; Gao, J.-F.; Song, P.; Shi, Y.-Q.; Tang, L.-C. Hydrophobic Silicone Modified Membranes for Efficient Oil/Water Separation: Synthesis, Fabrication and Application. *Sep. Purif. Technol.* **2025**, *353*, 128485. <https://doi.org/10.1016/j.seppur.2024.128485>.
- (238) Pan, L.-Q.; Zheng, Q.-N.; Feng, Q.-H.; Shen, Y.-B.; Hu, W.-Y.; Cao, C.-F.; Zhang, G.-D.; Gao, J.-F.; Song, P.; Shi, Y.-Q.; Tang, L.-C. Hydrophobic Silicone Modified Membranes for Efficient Oil/Water Separation: Synthesis, Fabrication and Application. *Sep. Purif. Technol.* **2025**, *353*, 128485. <https://doi.org/10.1016/j.seppur.2024.128485>.
- (239) Zhao, J.; Luo, G.; Wu, J.; Xia, H. Preparation of Microporous Silicone Rubber Membrane with Tunable Pore Size via Solvent Evaporation-Induced Phase Separation. *ACS Appl. Mater. Interfaces* **2013**, *5* (6), 2040–2046. <https://doi.org/10.1021/am302929c>.
- (240) Gutierrez, D. B.; Caldon, E. B.; Yang, Z.; Suo, X.; Cheng, X.; Dai, S.; Espiritu, R. D.; Advincula, R. C. 3D-Printed PDMS-Based Membranes for CO<sub>2</sub> Separation Applications. *MRS Commun.* **2022**, *12* (6), 1174–1182. <https://doi.org/10.1557/s43579-022-00287-1>.
- (241) Gutierrez, D. B.; Caldon, E. B.; Espiritu, R. D.; Advincula, R. C. The Potential of Additively Manufactured Membranes for Selective Separation and Capture of CO<sub>2</sub>. *MRS Commun.* **2021**, *11* (4), 391–401. <https://doi.org/10.1557/s43579-021-00062-8>.
- (242) Gutierrez, D. B.; Caldon, E. B.; Yang, Z.; Suo, X.; Cheng, X.; Dai, S.; Espiritu, R. D.; Advincula, R. C. PDMS-Silica Composite Gas Separation Membranes by Direct Ink Writing. *J. Appl. Polym. Sci.* **2023**, *140* (33), e54277. <https://doi.org/10.1002/app.54277>.
- (243) Espera, A. H.; Dizon, J. R. C.; Valino, A. D.; Chen, Q.; Silva, I. G. M.; Nguyen, D. V.; Rong, L.; Advincula, R. C. On the 3D Printability of Silicone-Based Adhesives via Viscous Paste Extrusion. *MRS Commun.* **2023**, *13* (1), 102–110. <https://doi.org/10.1557/s43579-022-00318-x>.
- (244) Elahee, G. M. F.; Cheng, X.; Rong, L.; Xu, M.-W.; Souza, L.; Advincula, R. C.; Maia, J. On the Cogent Formulation of an Elastomeric Silicone Ink Material for Direct Ink Write (DIW) 3D Printing. *Polym. Eng. Sci.* **2024**, *64* (6), 2476–2490. <https://doi.org/10.1002/pen.26703>.
- (245) Elahee, G. M. F.; Cheng, X.; De Souza, L. R.; Caldon, E. B.; Maia, J.; Advincula, R. C. Optimization in 3D Printable Silicone DIW Ink Formulations: Gelling Behavior Control and the Use of Carbon Nanotubes. *J. Appl. Polym. Sci.* *n/a* (n/a), e70442. <https://doi.org/10.1002/app.70442>.
- (246) Palaganas, J.; de Leon, A. C.; Mangadlao, J.; Palaganas, N.; Mael, A.; Lee, Y. J.; Lai, H. Y.; Advincula, R. Facile Preparation of Photocurable Siloxane Composite for 3D Printing. *Macromol. Mater. Eng.* **2017**, *302* (5), 1600477. <https://doi.org/10.1002/mame.201600477>.
- (247) Mondal, K.; Kaur, G.; Advincula, R. C. Advanced Silicone Materials for Soft Actuator Applications. *RSC Appl. Polym.* **2026**, *4* (1), 12–29. <https://doi.org/10.1039/D5LP00290G>.
- (248) Espino, M. T.; Tuazon, B. J.; Espera, A. H.; Nocheseda, C. J. C.; Manalang, R. S.; Dizon, J. R. C.; Advincula, R. C. Statistical Methods for Design and Testing of 3D-Printed

- Polymers. *MRS Commun.* **2023**, *13* (2), 193–211.  
<https://doi.org/10.1557/s43579-023-00332-7>.
- (249) Dizon, J. R. C.; Valino, A. D.; Souza, L. R.; Espera, A. H.; Chen, Q.; Advincula, R. C. Three-Dimensional-Printed Molds and Materials for Injection Molding and Rapid Tooling Applications. *MRS Commun.* **2019**, *9* (4), 1267–1283.  
<https://doi.org/10.1557/mrc.2019.147>.
- (250) Dizon, J. R. C.; Valino, A. D.; Souza, L. R.; Espera, A. H.; Chen, Q.; Advincula, R. C. 3D Printed Injection Molds Using Various 3D Printing Technologies. *Mater. Sci. Forum* **2020**, *1005*, 150–156. <https://doi.org/10.4028/www.scientific.net/MSF.1005.150>.
- (251) Smith, Z. J.; Barsoum, D. R.; Arwood, Z. L.; Penumadu, D.; Advincula, R. C. Characterization of Micro-Sandwich Structures via Direct Ink Writing Epoxy Based Cores. *J. Sandw. Struct. Mater.* **2023**, *25* (1), 112–127.  
<https://doi.org/10.1177/10996362221118329>.
- (252) Nanocomposite Membranes. In *Emerging Technologies for Sustainable Desalination Handbook*; Butterworth-Heinemann, 2018; pp 285–330.  
<https://doi.org/10.1016/B978-0-12-815818-0.00009-6>.
- (253) Manapat, J. Z.; Chen, Q.; Ye, P.; Advincula, R. C. 3D Printing of Polymer Nanocomposites via Stereolithography. *Macromol. Mater. Eng.* **2017**, *302* (9), 1600553.  
<https://doi.org/10.1002/mame.201600553>.
- (254) Palaganas, N. B.; Mangadlao, J. D.; de Leon, A. C. C.; Palaganas, J. O.; Pangilinan, K. D.; Lee, Y. J.; Advincula, R. C. 3D Printing of Photocurable Cellulose Nanocrystal Composite for Fabrication of Complex Architectures via Stereolithography. *ACS Appl. Mater. Interfaces* **2017**, *9* (39), 34314–34324. <https://doi.org/10.1021/acsami.7b09223>.
- (255) Manapat, J. Z.; Mangadlao, J. D.; Tiu, B. D. B.; Tritchler, G. C.; Advincula, R. C. High-Strength Stereolithographic 3D Printed Nanocomposites: Graphene Oxide Metastability. *ACS Appl. Mater. Interfaces* **2017**, *9* (11), 10085–10093.  
<https://doi.org/10.1021/acsami.6b16174>.
- (256) Maalihan, R. D.; Chen, Q.; Agueda, J. R. H. Sta.; Pajarito, B. B.; Tamura, H.; Advincula, R. C. On the Use of Surfactant-Complexed Chitosan for Toughening 3D Printed Polymethacrylate Composites. *Macromol. Mater. Eng.* **2021**, *306* (1), 2000448.  
<https://doi.org/10.1002/mame.202000448>.
- (257) Garcia, V. J.; Cheng, X.; Rong, L.; Lara-Ceniceros, T. E.; Ricohermoso, E.; Bonilla-Cruz, J.; Espiritu, R. D.; Advincula, R. C. Thermomechanical Properties of Stereolithographic 3D-Printed Zinc Oxide Nanocomposites. *MRS Commun.* **2024**, *14* (4), 676–685.  
<https://doi.org/10.1557/s43579-024-00602-y>.
- (258) Maalihan, R. D.; Pajarito, B. B.; Advincula, R. C. 3D-Printing Methacrylate/Chitin Nanowhiskers Composites via Stereolithography: Mechanical and Thermal Properties. *Mater. Today Proc.* **2020**, *33*, 1819–1824. <https://doi.org/10.1016/j.matpr.2020.05.063>.
- (259) Chen, Q.; Sukmanee, T.; Rong, L.; Yang, M.; Ren, J.; Ekgasit, S.; Advincula, R. A Dual Approach in Direct Ink Writing of Thermally Cured Shape Memory Rubber Toughened Epoxy. *ACS Appl. Polym. Mater.* **2020**, *2* (12), 5492–5500.  
<https://doi.org/10.1021/acsapm.0c00839>.
- (260) Demchuk, Z.; Zhu, J.; Li, B.; Zhao, X.; Islam, N. Md.; Bocharova, V.; Yang, G.; Zhou, H.; Jiang, Y.; Choi, W.; Advincula, R.; Cao, P.-F. Unravelling the Influence of Surface Modification on the Ultimate Performance of Carbon Fiber/Epoxy Composites. *ACS Appl. Mater. Interfaces* **2022**, *14* (40), 45775–45787. <https://doi.org/10.1021/acsami.2c11281>.

- (261) Khatri, N. R.; Islam, Md. N.; Cao, P.-F.; Advincula, R. C.; Choi, W.; Jiang, Y. Integrating Helicoid Channels for Passive Control of Fiber Alignment in Direct-Write 3D Printing. *Addit. Manuf.* **2021**, *48*, 102419. <https://doi.org/10.1016/j.addma.2021.102419>.
- (262) Chen, Q.; Mangadlao, J. D.; Wallat, J.; De Leon, A.; Pokorski, J. K.; Advincula, R. C. 3D Printing Biocompatible Polyurethane/Poly(Lactic Acid)/Graphene Oxide Nanocomposites: Anisotropic Properties. *ACS Appl. Mater. Interfaces* **2017**, *9* (4), 4015–4023. <https://doi.org/10.1021/acsami.6b11793>.
- (263) Memisoglu, G.; Murugesan, R. C.; Zubia, J.; Rozhin, A. G. Graphene Nanocomposite Membranes: Fabrication and Water Treatment Applications. *Membranes* **2023**, *13* (2), 145. <https://doi.org/10.3390/membranes13020145>.
- (264) Sta. Agueda, J. R. H.; Chen, Q.; Maalihan, R. D.; Ren, J.; da Silva, Í. G. M.; Dugos, N. P.; Caldon, E. B.; Advincula, R. C. 3D Printing of Biomedically Relevant Polymer Materials and Biocompatibility. *MRS Commun.* **2021**, *11* (2), 197–212. <https://doi.org/10.1557/s43579-021-00038-8>.
- (265) Yang, J.; Wang, Y.; Angelopoulou, P. P.; Keum, J.; Park, J.; Chen, J.; Advincula, R. C. 3D Printing of Polyelectrolyte Complex-Integrated Photocurable Hydrogel Resins. *ACS Appl. Polym. Mater.* **2025**, *7* (23), 15917–15927. <https://doi.org/10.1021/acsapm.5c03018>.
- (266) Castillo, A. E.; Trejo-Maldonado, M.; Lara-Ceniceros, T. E.; Ramírez-Soria, E. H.; Torres-Lubián, J. R.; Garza-Navarro, M. A.; Advincula, R. C.; Bonilla-Cruz, J. 3D-Printed PEGMA-Co-(PNIPAM Crosslinked with PEGDA) Hydrogels by Digital Light Processing in Aqueous Media. *MRS Commun.* **2025**, *15* (3), 320–330. <https://doi.org/10.1557/s43579-025-00732-x>.
- (267) Nguyen, A.; Jurago, A. A.; Viers, R. A.; Patten, C.; Chen, Q.; Caldon, E. B.; Advincula, R. C. 3D-Printing Formulated Polyelectrolyte Complexes (PECs) in Air: Silica Compositions in Rheological Optimization for Layering. *MRS Commun.* **2023**, *13* (6), 1326–1334. <https://doi.org/10.1557/s43579-023-00457-9>.
- (268) Jurago, A. A.; Viers, R. A.; Nguyen, A. T.; Ribeiro, E. L.; Espera, A. H.; Caldon, E. B.; Advincula, R. C. On the 3D Printing of Polyelectrolyte Complexes: A Novel Approach to Overcome Rheology Constraints. *MRS Commun.* **2023**, *13* (5), 862–870. <https://doi.org/10.1557/s43579-023-00415-5>.
- (269) Maalihan, R. D.; Chen, Q.; Tamura, H.; Sta. Agueda, J. R. H.; Pajarito, B. B.; Caldon, E. B.; Advincula, R. C. Mechanically and Thermally Enhanced 3D-Printed Photocurable Polymer Nanocomposites Containing Functionalized Chitin Nanowhiskers by Stereolithography. *ACS Appl. Polym. Mater.* **2022**, *4* (4), 2513–2526. <https://doi.org/10.1021/acsapm.1c01816>.
- (270) Radu, E. R.; Voicu, S. I.; Thakur, V. K. Polymeric Membranes for Biomedical Applications. *Polymers* **2023**, *15* (3), 619. <https://doi.org/10.3390/polym15030619>.
- (271) de Leon, A. C.; Rodier, B. J.; Bajamundi, C.; Espera, A. Jr.; Wei, P.; Kwon, J. G.; Williams, J.; Ilijasic, F.; Advincula, R. C.; Pentzer, E. Plastic Metal-Free Electric Motor by 3D Printing of Graphene-Polyamide Powder. *ACS Appl. Energy Mater.* **2018**, *1* (4), 1726–1733. <https://doi.org/10.1021/acsae.8b00240>.
- (272) Liu, J.; Hou, X.; Park, H. B.; Lin, H. High-Performance Polymers for Membrane CO<sub>2</sub>/N<sub>2</sub> Separation. *Chem. – Eur. J.* **2016**, *22* (45), 15980–15990. <https://doi.org/10.1002/chem.201603002>.

- (273) Dizon, J. R. C.; Espera, A. H.; Chen, Q.; Advincula, R. C. Mechanical Characterization of 3D-Printed Polymers. *Addit. Manuf.* **2018**, *20*, 44–67. <https://doi.org/10.1016/j.addma.2017.12.002>.
- (274) Huang, K.; Rowe, P.; Chi, C.; Sreepal, V.; Bohn, T.; Zhou, K.-G.; Su, Y.; Prestat, E.; Pillai, P. B.; Cherian, C. T.; Michaelides, A.; Nair, R. R. Cation-Controlled Wetting Properties of Vermiculite Membranes and Its Promise for Fouling Resistant Oil–Water Separation. *Nat. Commun.* **2020**, *11* (1), 1097. <https://doi.org/10.1038/s41467-020-14854-4>.
- (275) Gaxiola-López, J. C.; Lara-Ceniceros, T. E.; Silva-Vidaurre, L. G.; Advincula, R. C.; Bonilla-Cruz, J. 3D Printed Parahydrophobic Surfaces as Multireaction Platforms. *Langmuir* **2022**, *38* (25), 7740–7749. <https://doi.org/10.1021/acs.langmuir.2c00788>.
- (276) Bonilla-Cruz, J.; Sy, J. A. C.; Lara-Ceniceros, T. E.; Gaxiola-López, J. C.; García, V.; Basilia, B. A.; Advincula, R. C. Superhydrophobic  $\mu$ -Pillars via Simple and Scalable SLA 3D-Printing: The Stair-Case Effect and Their Wetting Models. *Soft Matter* **2021**, *17* (32), 7524–7531. <https://doi.org/10.1039/D1SM00655J>.
- (277) Kang, G.; Cao, Y. Application and Modification of Poly(Vinylidene Fluoride) (PVDF) Membranes – A Review. *J. Membr. Sci.* **2014**, *463*, 145–165. <https://doi.org/10.1016/j.memsci.2014.03.055>.
- (278) Islam, Md. N.; Rupom, R. H.; Adhikari, P. R.; Demchuk, Z.; Popov, I.; Sokolov, A. P.; Wu, H. F.; Advincula, R. C.; Dahotre, N.; Jiang, Y.; Choi, W. Boosting Piezoelectricity by 3D Printing PVDF-MoS<sub>2</sub> Composite as a Conformal and High-Sensitivity Piezoelectric Sensor. *Adv. Funct. Mater.* **2023**, *33* (42), 2302946. <https://doi.org/10.1002/adfm.202302946>.
- (279) Islam, Md. N.; Smith, Z.; Rupom, R. H.; Rijal, R.; Demchuk, Z.; Dahotre, N.; Wu, H. F.; Advincula, R. C.; Choi, W.; Jiang, Y. Self-Sensing Composites via an Embedded 3D-Printed PVDF-MoS<sub>2</sub> Nanosensor for Structural Health Monitoring. *ACS Appl. Mater. Interfaces* **2025**, *17* (24), 36026–36033. <https://doi.org/10.1021/acsami.5c05683>.
- (280) Jiang, Y.; Islam, Md. N.; He, R.; Huang, X.; Cao, P.-F.; Advincula, R. C.; Dahotre, N.; Dong, P.; Wu, H. F.; Choi, W. Recent Advances in 3D Printed Sensors: Materials, Design, and Manufacturing. *Adv. Mater. Technol.* **2023**, *8* (2), 2200492. <https://doi.org/10.1002/admt.202200492>.
- (281) Rupom, R. H.; Islam, M. N.; Demchuk, Z.; Advincula, R.; Dahotre, N. B.; Jiang, Y.; Choi, W. Tailoring Piezoelectricity of 3D Printing PVDF-MoS<sub>2</sub> Nanocomposite via In Situ Induced Shear Stress. *ACS Appl. Nano Mater.* **2024**, *7* (19), 22714–22722. <https://doi.org/10.1021/acsanm.4c03695>.
- (282) Patiño Jaimes, K. Y.; Caldoná, E. B.; Kim, E. M.; Lambert, J.; Winn, E. C.; Ribeiro, E. L.; Jiang, Y.; Ferdousi, S.; Hicks, B.; Wang, Y.; Ivanov, I. N.; Advincula, R. C. Distinct Mechanism of Anti-Corrosion and Swelling-Adhesion Modeling of Low-Dimensional Nylon-Fluoropolymer Composite Coatings. *ACS Appl. Polym. Mater.* **2024**, *6* (6), 3049–3059. <https://doi.org/10.1021/acsapm.3c02335>.
- (283) Wang, X.-S.; Ji, Y.-L.; Zheng, P.-Y.; An, Q.-F.; Zhao, Q.; Lee, K.-R.; Qian, J.-W.; Gao, C.-J. Engineering Novel Polyelectrolyte Complex Membranes with Improved Mechanical Properties and Separation Performance. *J. Mater. Chem. A* **2015**, *3* (14), 7296–7303. <https://doi.org/10.1039/C4TA06477A>.
- (284) Durmaz, E. N.; Baig, M. I.; Willott, J. D.; de Vos, W. M. Polyelectrolyte Complex Membranes via Salinity Change Induced Aqueous Phase Separation. *ACS Appl. Polym. Mater.* **2020**, *2* (7), 2612–2621. <https://doi.org/10.1021/acsapm.0c00255>.

- (285) Porcel, C. H.; Schlenoff, J. B. Compact Polyelectrolyte Complexes: “Saloplastic” Candidates for Biomaterials. *Biomacromolecules* **2009**, *10* (11), 2968–2975. <https://doi.org/10.1021/bm900373c>.
- (286) Sciortino, F.; Mir, S. H.; Pakdel, A.; Oruganti, A.; Abe, H.; Witecka, A.; Shri, D. N. A.; Rydzek, G.; Ariga, K. Saloplastics as Multiresponsive Ion Exchange Reservoirs and Catalyst Supports. *J. Mater. Chem. A* **2020**, *8* (34), 17713–17724. <https://doi.org/10.1039/D0TA05901C>.
- (287) Yang, S.; Kim, E.; Choi, J.; Choi, Y.-S.; Kim, S.-K. Multinetwork Vitrimer for High-Temperature Polymer Electrolyte Membranes. *Chem. Eng. J.* **2025**, *509*, 161270. <https://doi.org/10.1016/j.cej.2025.161270>.
- (288) Górecki, R.; Bhaumik, S.; Qasem, E.; Loiola, L.; Emwas, A.-H.; Ntetsikas, K.; Hadjichristidis, N.; Nunes, S. P. Well-Defined Block Copolymer Vitrimer Membranes. *Small* **2025**, *21* (3), 2409139. <https://doi.org/10.1002/smll.202409139>.
- (289) Chen, Q.; Zhao, X.; Li, B.; Sokolov, A. P.; Tian, M.; Advincula, R. C.; Cao, P.-F. Exceptionally Recyclable, Extremely Tough, Vitrimer-like Polydimethylsiloxane Elastomers via Rational Network Design. *Matter* **2023**, *6* (10), 3378–3393. <https://doi.org/10.1016/j.matt.2023.05.020>.
- (290) Ye, C.; Voet, V. S. D.; Folkersma, R.; Loos, K. Robust Superamphiphilic Membrane with a Closed-Loop Life Cycle. *Adv. Mater.* **2021**, *33* (15), 2008460. <https://doi.org/10.1002/adma.202008460>.
- (291) Niu, W.; Zhang, Z.; Chen, Q.; Cao, P.-F.; Advincula, R. C. Highly Recyclable, Mechanically Isotropic and Healable 3D-Printed Elastomers via Polyurea Vitrimers. *ACS Mater. Lett.* **2021**, *3* (8), 1095–1103. <https://doi.org/10.1021/acsmaterialslett.1c00132>.
- (292) Zhu, J.; Zhao, S.; Luo, J.; Niu, W.; Damron, J. T.; Zhang, Z.; Rahman, M. A.; Arnould, M. A.; Saito, T.; Advincula, R.; Sokolov, A. P.; Sumpter, B. G.; Cao, P.-F. A Novel Dynamic Polymer Synthesis via Chlorinated Solvent Quenched Depolymerization. *CCS Chem.* **2022**, *5* (8), 1841–1853. <https://doi.org/10.31635/ccschem.022.202202362>.
- (293) Bran Anleu, P.; Le Pape, Y.; Chen, Q.; Advincula, R.; Sun, X.-G.; Felder, J. B.; Meyer, H. M.; Post, B. K.; Lance, M. J.; Paranthaman, M. P. An Innovative Carbonated Cementitious Material and Its Printability and Carbon Mineralization Capacity. *Prog. Addit. Manuf.* **2024**, *9* (2), 435–444. <https://doi.org/10.1007/s40964-023-00463-2>.
- (294) Leong, S. X.; Griesbach, C. E.; Zhang, R.; Darvish, K.; Zhao, Y.; Mandal, A.; Zou, Y.; Hao, H.; Bernales, V.; Aspuru-Guzik, A. Steering towards Safe Self-Driving Laboratories. *Nat. Rev. Chem.* **2025**, *9* (10), 707–722. <https://doi.org/10.1038/s41570-025-00747-x>.
- (295) Seifrid, M.; Pollice, R.; Aguilar-Granda, A.; Morgan Chan, Z.; Hotta, K.; Ser, C. T.; Vestfrid, J.; Wu, T. C.; Aspuru-Guzik, A. Autonomous Chemical Experiments: Challenges and Perspectives on Establishing a Self-Driving Lab. *Acc. Chem. Res.* **2022**, *55* (17), 2454–2466. <https://doi.org/10.1021/acs.accounts.2c00220>.
- (296) Low, A. K. Y.; Cheng, J. J. W.; Hippalgaonkar, K.; Ng, L. W. T. Self-Driving Laboratories: Translating Materials Science from Laboratory to Factory. *ACS Omega* **2025**, *10* (28), 29902–29908. <https://doi.org/10.1021/acsomega.5c02197>.
- (297) AK, N.; Kumar, S. Integration of 2D Nanoporous Membranes in Microfluidic Devices. *ACS Omega* **2024**, *9* (20), 22305–22312. <https://doi.org/10.1021/acsomega.4c01688>.
- (298) Ferreira Da Silva, R.; Moore Ii, R.; Mintz, B.; Advincula, R.; Alnajjar, A.; Baldwin, L.; Bridges, C.; Coffee, R.; Deelman, E.; Engelmann, C.; Etz, B.; Firestone, M.; Foster, I.; Ganesh, P.; Hamilton, L.; Huber, D.; Ivanov, I.; Jha, S.; Li, Y.; Liu, Y.; Lofstead, J.; Mandal,

- A.; Martin, H.; Mayer, T.; McDonnell, M.; Murugesan, V.; Nimer, S.; Rao, N.; Seifrid, M.; Taheri, M.; Taufer, M.; Vogiatzis, K. *Shaping the Future of Self-Driving Autonomous Laboratories Workshop*; ORNL/TM--2024/3714, 2481197; 2024; p ORNL/TM--2024/3714, 2481197. <https://doi.org/10.2172/2481197>.
- (299) Muckley, E. S.; Vasudevan, R.; Sumpter, B. G.; Advincula, R. C.; Ivanov, I. N. Machine Intelligence-Centered System for Automated Characterization of Functional Materials and Interfaces. *ACS Appl. Mater. Interfaces* **2023**, *15* (1), 2329–2340. <https://doi.org/10.1021/acscami.2c16088>.
- (300) Mukhin, N.; Jha, P.; Abolhasani, M. The Role of Flow Chemistry in Self-Driving Labs. *Matter* **2025**, *8* (7). <https://doi.org/10.1016/j.matt.2025.102205>.
- (301) Advincula, R.; Ivanov, I.; Vasudevan, R.; Kumar, R.; Christakopoulos, P.; Tsakanika, M.; Chen, J.; Michael Carillo, J.; Zhu, Q.; Sumpter, B. Harnessing Data and Control with AI/ML-Driven Polymerization and Copolymerization. *Faraday Discuss.* **2026**. <https://doi.org/10.1039/D5FD00066A>.
- (302) Bonciolini, S.; Pulcinella, A.; Noël, T. Tech-Enhanced Synthesis: Exploring the Synergy between Organic Chemistry and Technology. *J. Am. Chem. Soc.* **2025**, *147* (32), 28523–28545. <https://doi.org/10.1021/jacs.5c10303>.
- (303) Abolhasani, M.; Kumacheva, E. The Rise of Self-Driving Labs in Chemical and Materials Sciences. *Nat. Synth.* **2023**, *2* (6), 483–492. <https://doi.org/10.1038/s44160-022-00231-0>.
- (304) Tom, G.; Schmid, S. P.; Baird, S. G.; Cao, Y.; Darvish, K.; Hao, H.; Lo, S.; Pablo-García, S.; Rajaonson, E. M.; Skreta, M.; Yoshikawa, N.; Corapi, S.; Akkoc, G. D.; Strieth-Kalthoff, F.; Seifrid, M.; Aspuru-Guzik, A. Self-Driving Laboratories for Chemistry and Materials Science. *Chem. Rev.* **2024**, *124* (16), 9633–9732. <https://doi.org/10.1021/acs.chemrev.4c00055>.
- (305) Ignacz, G.; Beke, A. K.; Toth, V.; Szekely, G. A Hybrid Modelling Approach to Compare Chemical Separation Technologies in Terms of Energy Consumption and Carbon Dioxide Emissions. *Nat. Energy* **2025**, *10* (3), 308–317. <https://doi.org/10.1038/s41560-024-01668-7>.
- (306) Bouhid de Aguiar, I.; Schroën, K. Microfluidics Used as a Tool to Understand and Optimize Membrane Filtration Processes. *Membranes* **2020**, *10* (11), 316. <https://doi.org/10.3390/membranes10110316>.
- (307) Chen, X.; Shen, J. Review of Membranes in Microfluidics. *J. Chem. Technol. Biotechnol.* **2017**, *92* (2), 271–282. <https://doi.org/10.1002/jctb.5105>.
- (308) Bouhid de Aguiar, I.; Schroën, K. Microfluidics Used as a Tool to Understand and Optimize Membrane Filtration Processes. *Membranes* **2020**, *10* (11), 316. <https://doi.org/10.3390/membranes10110316>.
- (309) McIntyre, D.; Lashkaripour, A.; Fordyce, P.; Densmore, D. Machine Learning for Microfluidic Design and Control. *Lab. Chip* **2022**, *22* (16), 2925–2937. <https://doi.org/10.1039/D2LC00254J>.
- (310) Tao, X.; Naegele, T. E.; Rognin, E.; Willis-Fox, N.; Oldroyd, P.; Dong, C.; KISSOVSKY, S.; Dominguez-Alfaro, A.; Velasco-Bosom, S.; Daly, R.; Malliaras, G. G. Toolkit for Integrating Millimeter-Sized Microfluidic Biomedical Devices with Multiple Membranes and Electrodes. *Microsyst. Nanoeng.* **2025**, *11* (1), 33. <https://doi.org/10.1038/s41378-025-00871-0>.

- (311) Ali, I.; Messali, M.; Gogolashvili, A.; Giunashvili, L. Advances in Artificial Intelligence and Machine Learning in Capillary Electrophoresis. *Anal. Methods* **2025**, *17* (46), 9304–9318. <https://doi.org/10.1039/D5AY01500F>.
- (312) Tao, H.; Wu, T.; Kheiri, S.; Aldeghi, M.; Aspuru-Guzik, A.; Kumacheva, E. Self-Driving Platform for Metal Nanoparticle Synthesis: Combining Microfluidics and Machine Learning. *Adv. Funct. Mater.* **2021**, *31* (51), 2106725. <https://doi.org/10.1002/adfm.202106725>.
- (313) Yong, J.; Peng, Y.; Wang, X.; Li, J.; Hu, Y.; Chu, J.; Wu, D. Self-Driving Underwater “Aerofluidics.” *Adv. Sci.* **2023**, *10* (21), 2301175. <https://doi.org/10.1002/advs.202301175>.
- (314) Sadeghi, S.; Bateni, F.; Kim, T.; Son, D. Y.; Bennett, J. A.; Orouji, N.; Punati, V. S.; Stark, C.; Cerra, T. D.; Awad, R.; Delgado-Licona, F.; Xu, J.; Mukhin, N.; Dickerson, H.; Reyes, K. G.; Abolhasani, M. Autonomous Nanomanufacturing of Lead-Free Metal Halide Perovskite Nanocrystals Using a Self-Driving Fluidic Lab. *Nanoscale* **2024**, *16* (2), 580–591. <https://doi.org/10.1039/D3NR05034C>.
- (315) Chan, E. M. Automated Nanocrystal Synthesis: Lessons from 25 Years of Robots, Microfluidics, and Machine Learning. *Nano Lett.* **2026**, *26* (1), 8–17. <https://doi.org/10.1021/acs.nanolett.5c05228>.
- (316) Qi, X.; Hu, G. Harnessing Microfluidics for the Effective and Precise Synthesis of Advanced Materials. *Micromachines* **2025**, *16* (10), 1106. <https://doi.org/10.3390/mi16101106>.
- (317) Zhang, X.; Guo, J.; Wang, C. Predicting Real-Time Spectra from High-Speed Imaging: An Ultrafast Machine Vision Framework for Online Optical Control in Microfluidics. *Adv. Mater. Technol.* **2024**, *9* (15), 2101344. <https://doi.org/10.1002/admt.202101344>.
- (318) Nguyen, D.-N.; Tong, R. K.-Y.; Dinh, N.-D. DropMicroFluidAgents (DMFAs): Autonomous Droplet Microfluidic Research Framework through Large Language Model Agents. *Digit. Discov.* **2025**, *4* (10), 2827–2851. <https://doi.org/10.1039/D5DD00306G>.
- (319) Zhu, L.-T.; Chen, X.-Z.; Ouyang, B.; Yan, W.-C.; Lei, H.; Chen, Z.; Luo, Z.-H. Review of Machine Learning for Hydrodynamics, Transport, and Reactions in Multiphase Flows and Reactors. *Ind. Eng. Chem. Res.* **2022**, *61* (28), 9901–9949. <https://doi.org/10.1021/acs.iecr.2c01036>.
- (320) Lu, J.-M.; Wang, H.-F.; Guo, Q.-H.; Wang, J.-W.; Li, T.-T.; Chen, K.-X.; Zhang, M.-T.; Chen, J.-B.; Shi, Q.-N.; Huang, Y.; Shi, S.-W.; Chen, G.-Y.; Pan, J.-Z.; Lu, Z.; Fang, Q. Robotized AI-Assisted Microfluidic Photocatalytic Synthesis and Screening up to 10,000 Reactions per Day. *Nat. Commun.* **2024**, *15* (1), 8826. <https://doi.org/10.1038/s41467-024-53204-6>.
- (321) Jeraal, M. I.; Sung, S.; Lapkin, A. A. A Machine Learning-Enabled Autonomous Flow Chemistry Platform for Process Optimization of Multiple Reaction Metrics. *Chemistry–Methods* **2021**, *1* (1), 71–77. <https://doi.org/10.1002/cmtd.202000044>.
- (322) Volk, A. A.; Epps, R. W.; Yonemoto, D. T.; Masters, B. S.; Castellano, F. N.; Reyes, K. G.; Abolhasani, M. AlphaFlow: Autonomous Discovery and Optimization of Multi-Step Chemistry Using a Self-Driven Fluidic Lab Guided by Reinforcement Learning. *Nat. Commun.* **2023**, *14* (1), 1403. <https://doi.org/10.1038/s41467-023-37139-y>.
- (323) Chauhan, R.; Rana, A.; Santra, A.; Singh, A. K. Machine Learning for Efficient Substitution Control toward Azido-Substituted I-Sugar Synthesis via Flow Chemistry. *Org. Process Res. Dev.* **2025**, *29* (12), 3229–3235. <https://doi.org/10.1021/acs.oprd.5c00363>.

- (324) Dadfar, B.; Alemdag, B.; Kabay, G. The Alchemist, the Scientist, and the Robot: Exploring the Potential of Human-AI Symbiosis in Self-Driving Polymer Laboratories. *Macromol. Rapid Commun.* **2025**, *46* (23), e00380. <https://doi.org/10.1002/marc.202500380>.
- (325) Sumpter, B. G.; Hong, K.; Vasudevan, R. K.; Ivanov, I.; Advincula, R. Autonomous Continuous Flow Reactor Synthesis for Scalable Atom-Precision. *Carbon Trends* **2023**, *10*, 100234. <https://doi.org/10.1016/j.cartre.2022.100234>.
- (326) Ye, P.; Cao, P.-F.; Chen, Q.; Advincula, R. Continuous Flow Fabrication of Block Copolymer–Grafted Silica Micro-Particles in Environmentally Friendly Water/Ethanol Media. *Macromol. Mater. Eng.* **2019**, *304* (2), 1800451. <https://doi.org/10.1002/mame.201800451>.
- (327) Ye, P.; Cao, P.-F.; Su, Z.; Advincula, R. Highly Efficient Reversible Addition–Fragmentation Chain-Transfer Polymerization in Ethanol/Water via Flow Chemistry. *Polym. Int.* **2017**, *66* (9), 1252–1258. <https://doi.org/10.1002/pi.5374>.
- (328) Ge, J.; Yin, Y.; Caldon, E. B.; Advincula, R. C. Hyperbranched PDMAEMA-Functionalized SiO<sub>2</sub> Microparticles: ATRP Polymerization and Grafting in a Continuous Flow Reactor. *MRS Commun.* **2022**, *12* (6), 1147–1153. <https://doi.org/10.1557/s43579-022-00263-9>.
- (329) Rong, L.-H.; Cheng, X.; Ge, J.; Caldon, E. B.; Advincula, R. C. Synthesis of Hyperbranched Polymers via PET-RAFT Self-Condensing Vinyl Polymerization in a Flow Reactor. *Macromol. Chem. Phys.* **2022**, *223* (1), 2100342. <https://doi.org/10.1002/macp.202100342>.
- (330) Rong, L.-H.; Caldon, E. B.; Advincula, R. C. PET-RAFT Polymerization under Flow Chemistry and Surface-Initiated Reactions. *Polym. Int.* **2023**, *72* (2), 145–157. <https://doi.org/10.1002/pi.6475>.
- (331) Pittaway, P. M.; Knox, S. T.; Cayre, O. J.; Kapur, N.; Golden, L.; Drillieres, S.; Warren, N. J. Self-Driving Laboratory for Emulsion Polymerization. *Chem. Eng. J.* **2025**, *507*, 160700. <https://doi.org/10.1016/j.cej.2025.160700>.
- (332) Kumar, R.; Liu, Z.; Lokitz, B.; Chen, J.; Carrillo, J.-M.; Jakowski, J.; Collier, C. P.; Retterer, S.; Advincula, R. Harnessing Autocatalytic Reactions in Polymerization and Depolymerization. *MRS Commun.* **2021**, *11* (4), 377–390. <https://doi.org/10.1557/s43579-021-00061-9>.
- (333) Lo, S.; Baird, S. G.; Schrier, J.; Blaiszik, B.; Carson, N.; Foster, I.; Aguilar-Granda, A.; Kalinin, S. V.; Maruyama, B.; Politi, M.; Tran, H.; Sparks, T. D.; Aspuru-Guzik, A. Review of Low-Cost Self-Driving Laboratories in Chemistry and Materials Science: The “Frugal Twin” Concept. *Digit. Discov.* **2024**, *3* (5), 842–868. <https://doi.org/10.1039/D3DD00223C>.
- (334) Taylor, C. J.; Baker, A.; Chapman, M. R.; Reynolds, W. R.; Jolley, K. E.; Clemens, G.; Smith, G. E.; Blacker, A. J.; Chamberlain, T. W.; Christie, S. D. R.; Taylor, B. A.; Bourne, R. A. Flow Chemistry for Process Optimisation Using Design of Experiments. *J. Flow Chem.* **2021**, *11* (1), 75–86. <https://doi.org/10.1007/s41981-020-00135-0>.
- (335) Doloi, S.; Das, M.; Li, Y.; Cho, Z. H.; Xiao, X.; Hanna, J. V.; Osvaldo, M.; Tat, L. N. W. Democratizing Self-Driving Labs: Advances in Low-Cost 3D Printing for Laboratory Automation. *Digit. Discov.* **2025**, *4* (7), 1685–1721. <https://doi.org/10.1039/D4DD00411F>.
- (336) Price, A. J. N.; Capel, A. J.; Lee, R. J.; Pradel, P.; Christie, S. D. R. An Open Source Toolkit for 3D Printed Fluidics. *J. Flow Chem.* **2021**, *11* (1), 37–51. <https://doi.org/10.1007/s41981-020-00117-2>.

- (337) Leong, K. M.; Sun, A. Y.; Quach, M. L.; Lin, C. H.; Craig, C. A.; Guo, F.; Robinson, T. R.; Chang, M. M.; Olanrewaju, A. O. Democratizing Access to Microfluidics: Rapid Prototyping of Open Microchannels with Low-Cost LCD 3D Printers. *ACS Omega* **2024**, *9* (45), 45537–45544. <https://doi.org/10.1021/acsomega.4c07776>.
- (338) Tabassum, T.; Iloska, M.; Scuereb, D.; Taira, N.; Jin, C.; Zaitsev, V.; Afshar, F.; Kim, T. Development and Application of 3D Printed Mesoreactors in Chemical Engineering Education. *J. Chem. Educ.* **2018**, *95* (5), 783–790. <https://doi.org/10.1021/acs.jchemed.7b00663>.
- (339) Fan, Y.; Feng, X. Rising Millifluidics: A Practical Approach Towards Wide Application. *Crit. Rev. Anal. Chem.* **2025**, *0* (0), 1–19. <https://doi.org/10.1080/10408347.2025.2592579>.
- (340) Zhang, Y.; Li, M.; Tseng, T.-M.; Schlichtmann, U. Open-Source Interactive Design Platform for 3D-Printed Microfluidic Devices. *Commun. Eng.* **2024**, *3* (1), 71. <https://doi.org/10.1038/s44172-024-00217-0>.
- (341) Goenner, B.; Temple, S.; Zapata, S.; Wakeham, D.; Snelgrove, A.; Gaillardon, P.-E.; Nordin, G. P.; Gale, B. K. An Open Source Platform to Automate the Design, Verification, and Manufacture of 3D Printed Microfluidic Devices. *Sci. Rep.* **2025**, *15* (1), 33077. <https://doi.org/10.1038/s41598-025-15976-9>.
- (342) Sun, A. Y.; Lin, C. H.; Tatka, J. A.; Drake, K.; Daily, S.; Castellanos, M.; Nelson, A.; Olanrewaju, A. O. 3D Printing of Low-Cost, High-Resolution Open Capillary Microfluidics towards Self-Sustaining, Long-Term Hydration of Engineered Living Materials. *Prog. Addit. Manuf.* **2025**, *10* (10), 7927–7934. <https://doi.org/10.1007/s40964-025-01081-w>.
- (343) König, B.; Kreitmeier, P.; Hilgers, P.; Wirth, T. Flow Chemistry in Undergraduate Organic Chemistry Education. *J. Chem. Educ.* **2013**, *90* (7), 934–936. <https://doi.org/10.1021/ed3006083>.
- (344) Allemann, C.; Marti, R. Education in Flow Chemistry. *CHIMIA* **2023**, *77* (5), 294–299. <https://doi.org/10.2533/chimia.2023.294>.
- (345) Penny, M. R.; Tsui, N.; Hilton, S. T. Extending Practical Flow Chemistry into the Undergraduate Curriculum via the Use of a Portable Low-Cost 3D Printed Continuous Flow System. *J. Flow Chem.* **2021**, *11* (1), 19–29. <https://doi.org/10.1007/s41981-020-00122-5>.
- (346) Renner, M.; Griesbeck, A. Think and Print: 3D Printing of Chemical Experiments. *J. Chem. Educ.* **2020**, *97* (10), 3683–3689. <https://doi.org/10.1021/acs.jchemed.0c00416>.
- (347) Liu, Y.; Lei, Q.; He, X.; Xue, Y.; He, K.; Yang, H.; Wang, Y.; Zhang, X.; Yang, L.; Zhou, Y.; Hu, R.; Xie, Y. Building an Affordable Self-Driving Lab: Practical Machine Learning Experiments for Physics Education Using Internet-of-Things. *APL Mach. Learn.* **2025**, *3* (4), 046105. <https://doi.org/10.1063/5.0283529>.
- (348) Dougher, M.; Lair, L.; Ouimet, J. A.; Phillip, W. A.; Tarka, T. J.; Dowling, A. W. Opportunities for Process Intensification with Membranes to Promote Circular Economy Development for Critical Minerals. *Syst. Control Trans.* **2024**, 127504.
- (349) Middleton, A.; Hsu-Kim, H. Separation of Rare-Earth Elements by Supported Liquid Membranes: Impacts of Soluble Iron, Aluminum, and pH in Low-Grade Feedstocks. *ACS EST Eng.* **2023**, *3* (8), 1197–1204. <https://doi.org/10.1021/acsestengg.3c00060>.
- (350) Saidi, P.; Béland, L. K.; Daymond, M. R. Graphene Oxide Membranes for Water Isotope Filtration: Insight at the Nano- and Microscale. *J. Phys. Chem. C* **2020**, *124* (49), 26864–26873. <https://doi.org/10.1021/acs.jpcc.0c08817>.

- (351) Bhowmick, S.; Hernández, M. I.; Campos-Martínez, J.; Suleimanov, Y. V. Isotopic Separation of Helium through Graphyne Membranes: A Ring Polymer Molecular Dynamics Study. *Phys. Chem. Chem. Phys.* **2021**, *23* (34), 18547–18557. <https://doi.org/10.1039/D1CP02121D>.
- (352) Iordache, A. M.; Nasture, A. M.; Zgavarogea, R.; Andrei, R.; Mandoc, R.; Feizula, E.; Santos, R.; Nechita, C. Lithium Isotope Separation Using the 15-Crown-5 Ether System and Laboratory-Made Membranes. *Materials* **2025**, *18* (9), 2016. <https://doi.org/10.3390/ma18092016>.
- (353) Abels, C.; Carstensen, F.; Wessling, M. Membrane Processes in Biorefinery Applications. *J. Membr. Sci.* **2013**, *444*, 285–317. <https://doi.org/10.1016/j.memsci.2013.05.030>.
- (354) Membrane Processes and Applications for Biorefineries. In *Current Trends and Future Developments on (Bio-) Membranes*; Elsevier, 2020; pp 283–301. <https://doi.org/10.1016/B978-0-12-816778-6.00013-8>.
- (355) Polymeric Membranes in Biorefinery. In *Membrane Technologies for Biorefining*; Woodhead Publishing, 2016; pp 29–59. <https://doi.org/10.1016/B978-0-08-100451-7.00002-5>.
- (356) Nielsen, C. H. Biomimetic Membranes for Sensor and Separation Applications. *Anal. Bioanal. Chem.* **2009**, *395* (3), 697–718. <https://doi.org/10.1007/s00216-009-2960-0>.
- (357) Liu, X.; Zhang, G.; Mohawes, K. B. A.; Khashab, N. M. Smart Membranes for Separation and Sensing. *Chem. Sci.* **2024**, *15* (45), 18772–18788. <https://doi.org/10.1039/D4SC04793A>.

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