An AI-Guided Approach to Tuning Block Copolymer Nanostructures Through Homopolymer Incorporation for Advancing Filtration and Energy Storage Applications

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Many advanced technologies, from water purification membranes to battery electrolytes, rely on block copolymers (BCPs) because they can self-assemble into well-defined nanoscale morphologies, which directly impact the materials' performance in these applications. However, controlling specific morphology tailored to these applications typically requires synthesizing new polymers, which is time-consuming. This work offers a strategy for tuning BCP morphology by blending homopolymers and using an AI-driven framework for precise control of domain spacing and structural ordering. Polystyrene-b-poly(4-vinylpyridine) was blended with polystyrene homopolymers of two molecular weights across various compositions. Thin films were created by spin coating onto surface-treated silicon wafers. Then, nanoscale morphologies were characterized using Grazing-Incidence Small-Angle X-ray Scattering (GISAXS) measurements provided by a national laboratory and Atomic Force Microscopy (AFM) imaging. GISAXS measurements were further analyzed using Python-based peak fitting to extract domain spacing and full width at half maximum, while AFM images visualized local morphology. To efficiently identify homopolymer compositions that achieve both a target domain spacing and high structural ordering, a Gaussian process–based Bayesian optimization framework was employed, using uncertainty estimates to balance exploration and exploitation within the compositional space. Results of this study show that blend ratio primarily controls domain spacing and ordering, and higher molecular weight homopolymers increase sensitivity to compositional changes. Overall, this study shows that homopolymer blending, combined with an AI-framework, provides a predictive pathway to tune BCP morphology.

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