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**STRUCTURE OF ANION-CONDUCTING POLYMERS
FROM WAXS AND MD SIMULATIONS**

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— The structure of novel polymers for anion exchange membranes (AEMs) is investigated using wide angle X-ray scattering (WAXS) combined with molecular dynamics (MD) simulations using a united-atom force field model based on the DREIDING force field. The polymers being studied are poly(benzimidazole) (PBI) derivatives including poly(dimethylbenzimidazole) (PDMBI), mesitylene poly(benzimidazole) (mes-PBI), and mesitylene poly(dimethylbenzimidazole) (mes-PDMBI). WAXS reveals an amorphous structure with two main length scales. By comparing simulation results to WAXS data, we attribute features observed in the scattering data to side-to-side spacing between polymer chains and to the parallel-ring stacking of the benzimidazole rings. Overall, we are able to validate the interpretation of scattering data by combining MD simulations and scattering experiments.

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