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Supporting Information

Decoding Molecular Weight Effects in Polyimide Membranes for CO_2/CH_4 Separation: Bridging Experiments and Simulations

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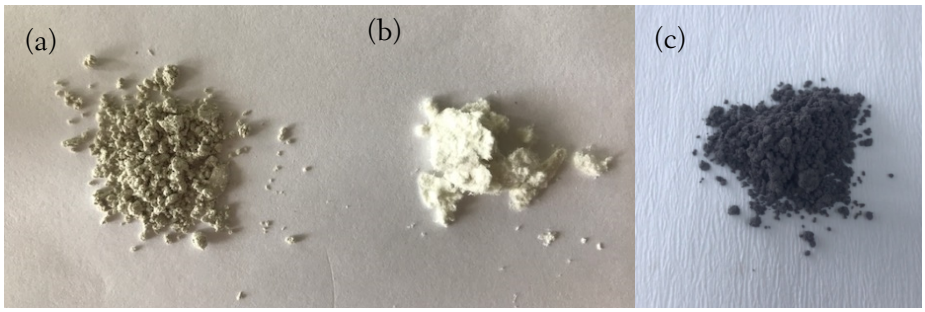


Figure S1. Photographic comparison illustrating the purification of the DABA monomer: (a) as-received commercial DABA displaying noticeable grayish-brown discoloration caused by trace air-oxidation and quinoid-type by-products, (b) recrystallized DABA displaying pure off-white needle-like crystals following activated carbon treatment, and (c) darkened DABA under standard storage conditions due to air oxidation.

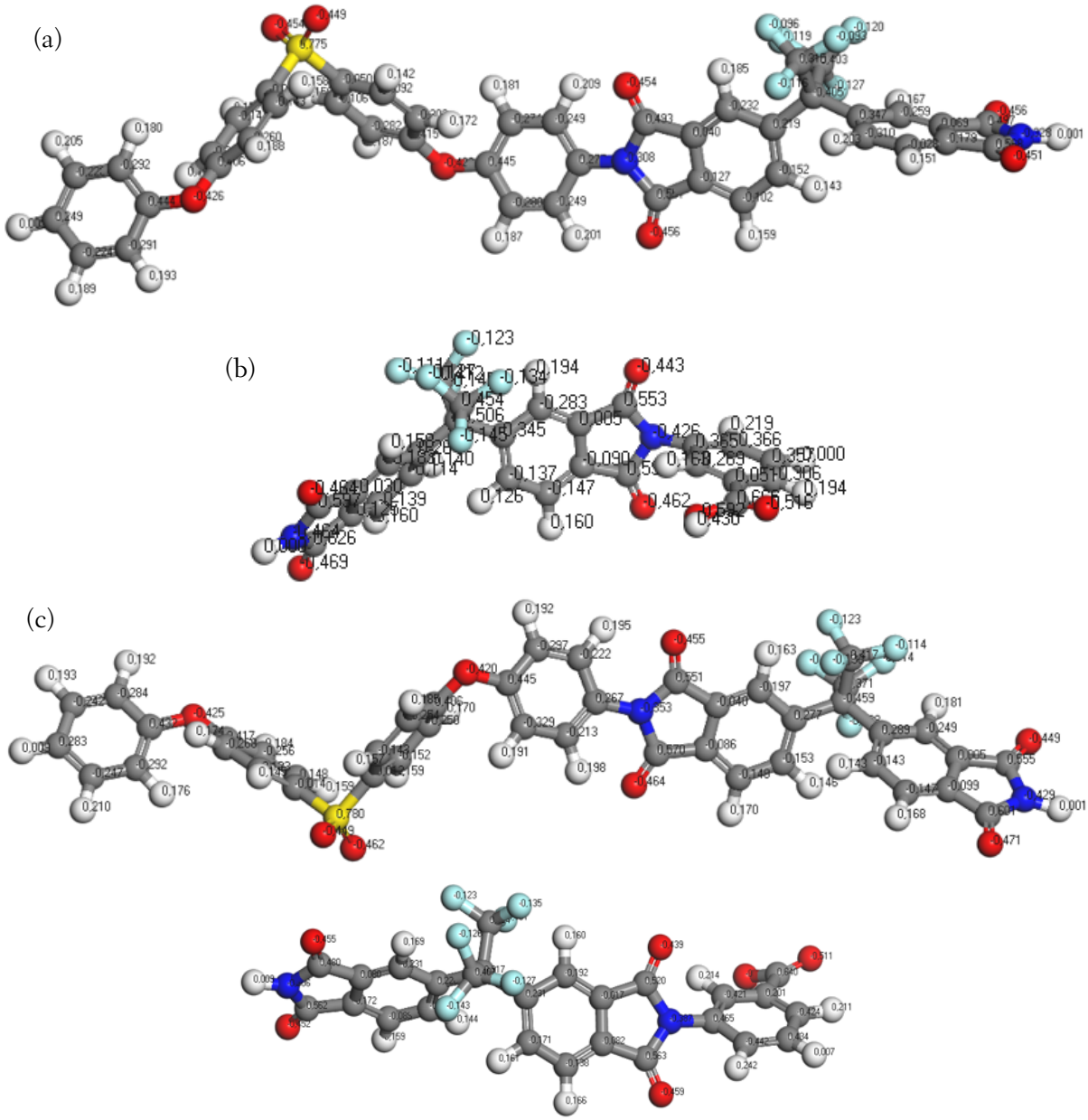


Figure S2. Partial charge distributions in (a) 6FDA-pBAPS, (b) 6FDA-DABA, and (c) 6FDA-pBAPS/DABA (3/1) units (C: gray, O: red, N: blue, H: white, F: turquoise, S: yellow).

Table S1. Adsorption sites investigated on polyimide monomers for RDF analysis.

Monomer	Designation	Description
6FDA	N1	nitrogen in the imide ring
6FDA	O1	oxygen in the carbonyl group
6FDA	F1	fluorine in the $-CF_3$ side groups
DABA	O2	oxygen in the carboxylic acid group
*p*BAPS	O3	oxygen linkage in the backbone
*p*BAPS	S1	sulfur linkage in

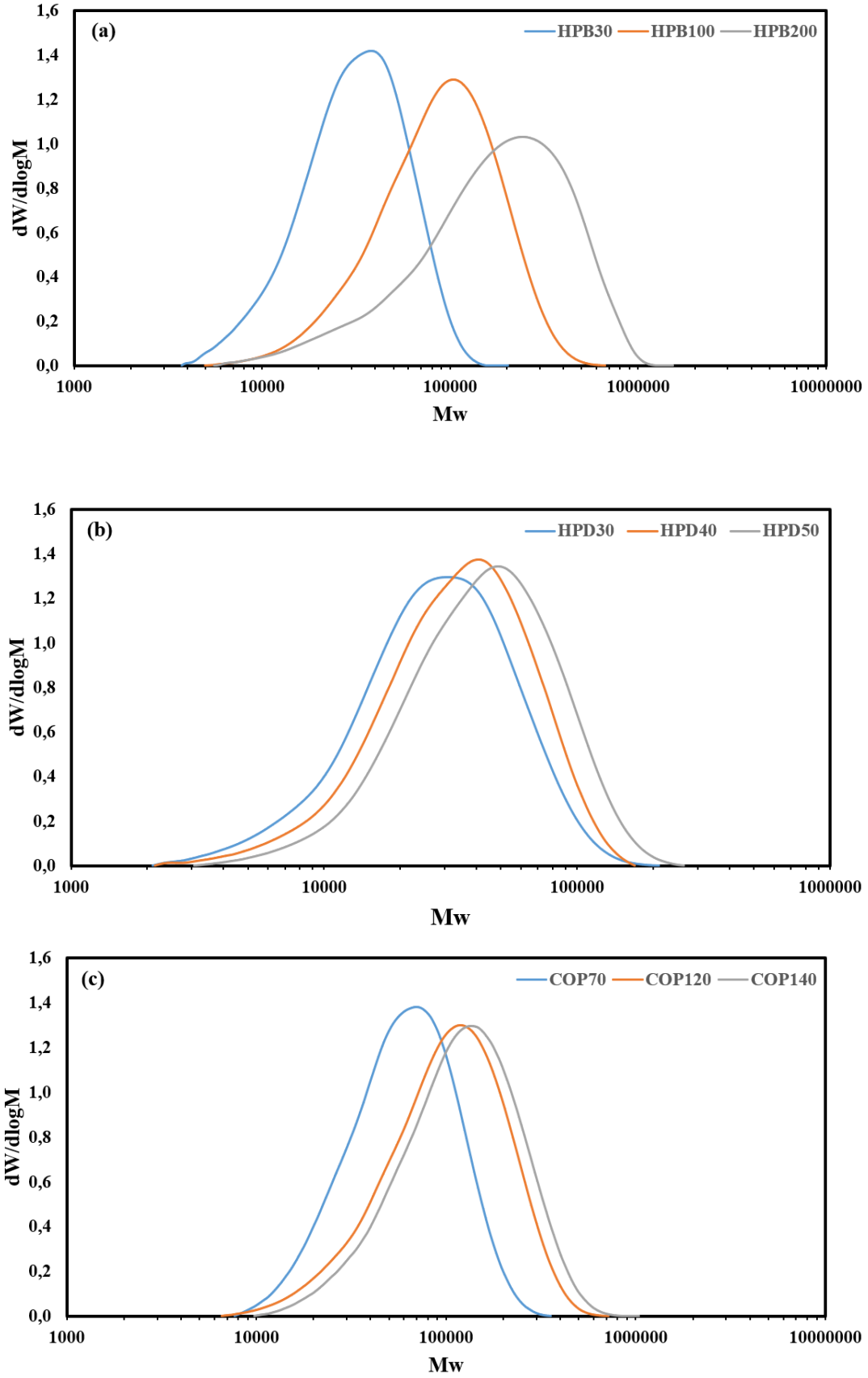


Figure S3. M_w distribution plots of different molecular weight polymers. (a) 6FDA-*p*BAPS, (b) 6FDA-DABA, and (c) 6FDA-*p*BAPS/DABA (3/1).

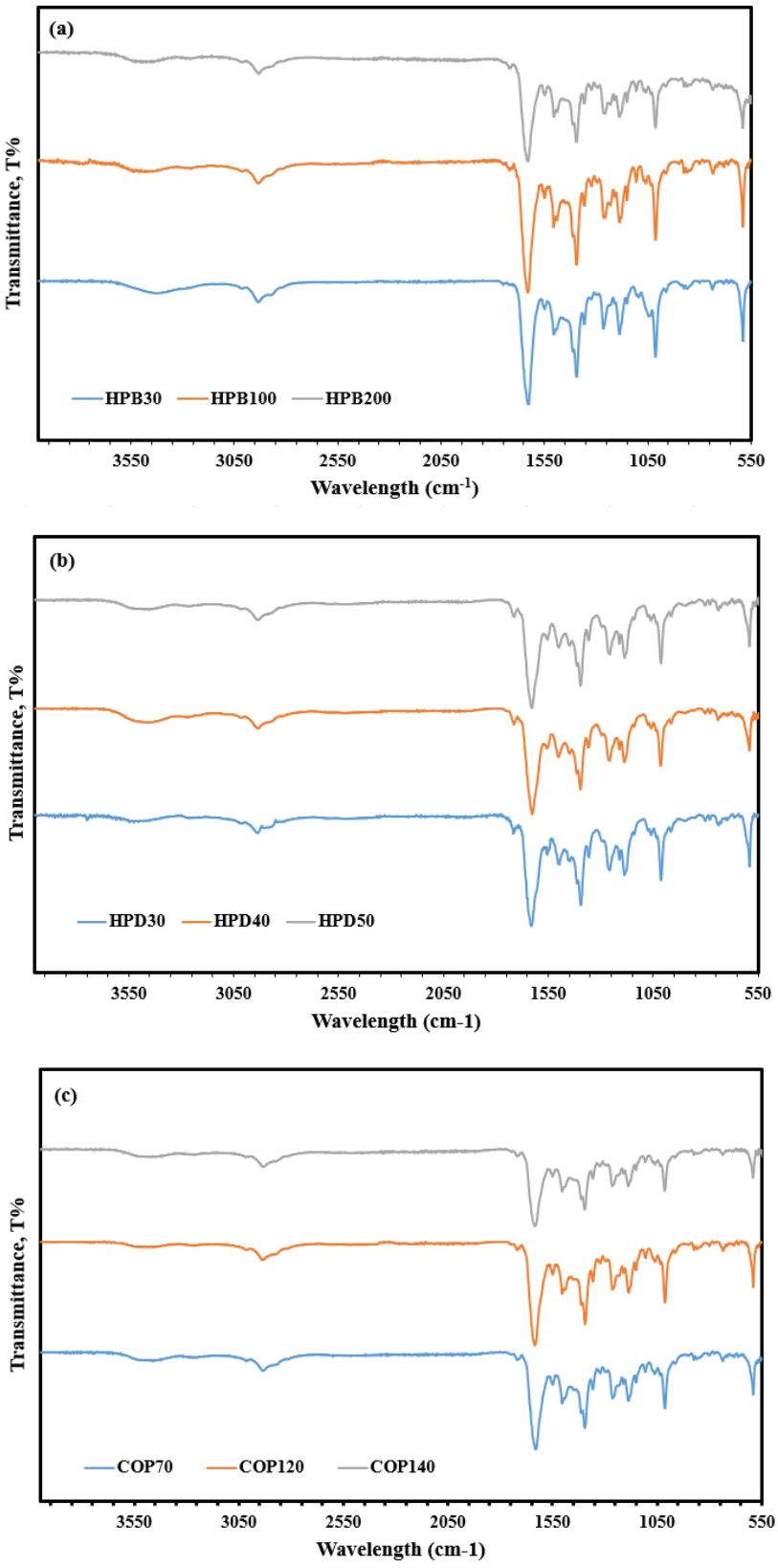


Figure S4. FTIR-ATR spectra of polyamic acids of different molecular weight polymers. (a) 6FDA-pBAPS, (b) 6FDA-DABA, and (c) 6FDA-pBAPS/DABA (3/1).

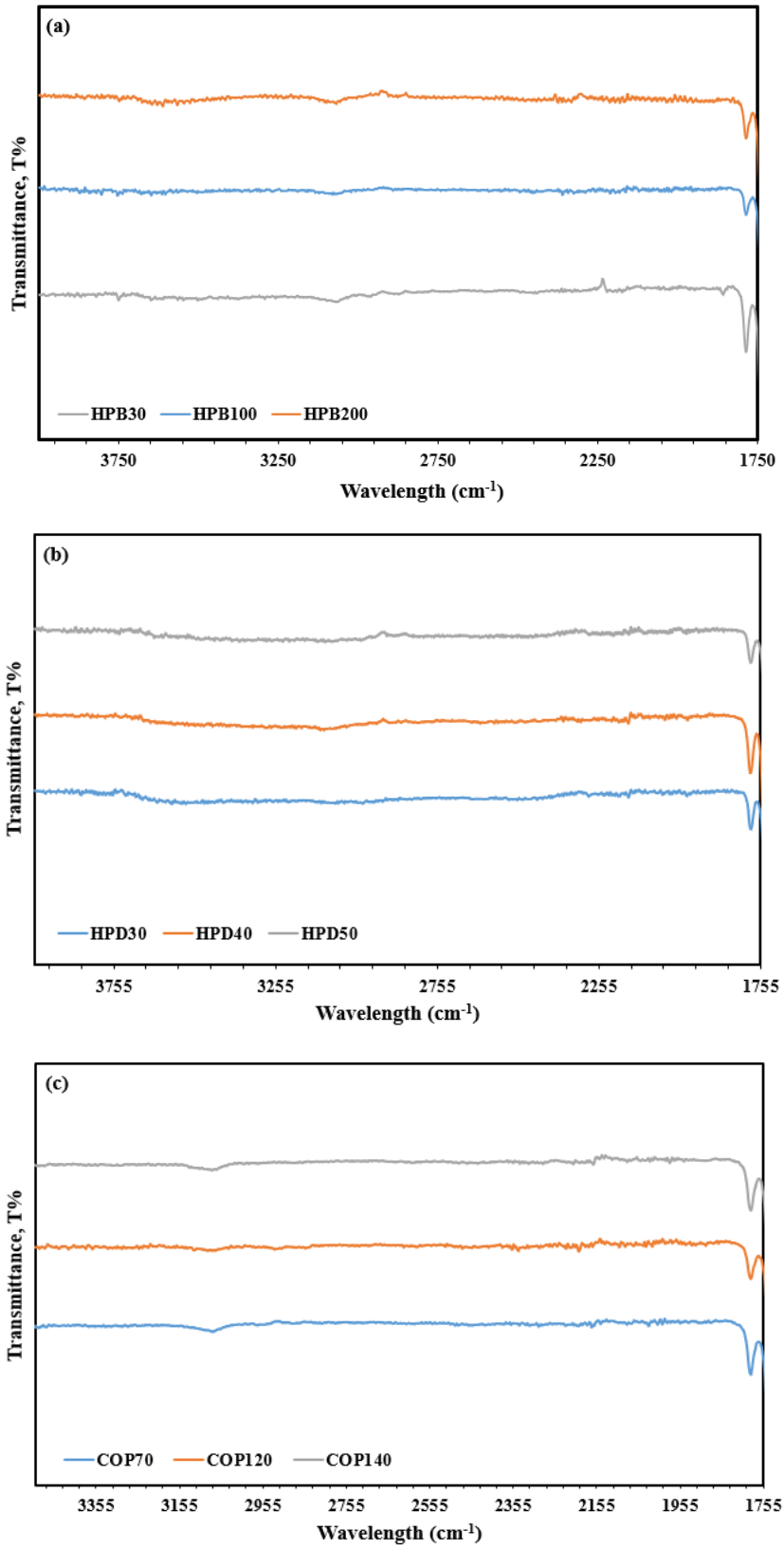


Figure S5. FTIR-ATR spectra of polyimides between 1755-4000 cm^{-1}. (a) 6FDA-pBAPS, (b) 6FDA-DABA, and (c) 6FDA-pBAPS/DABA (3/1).

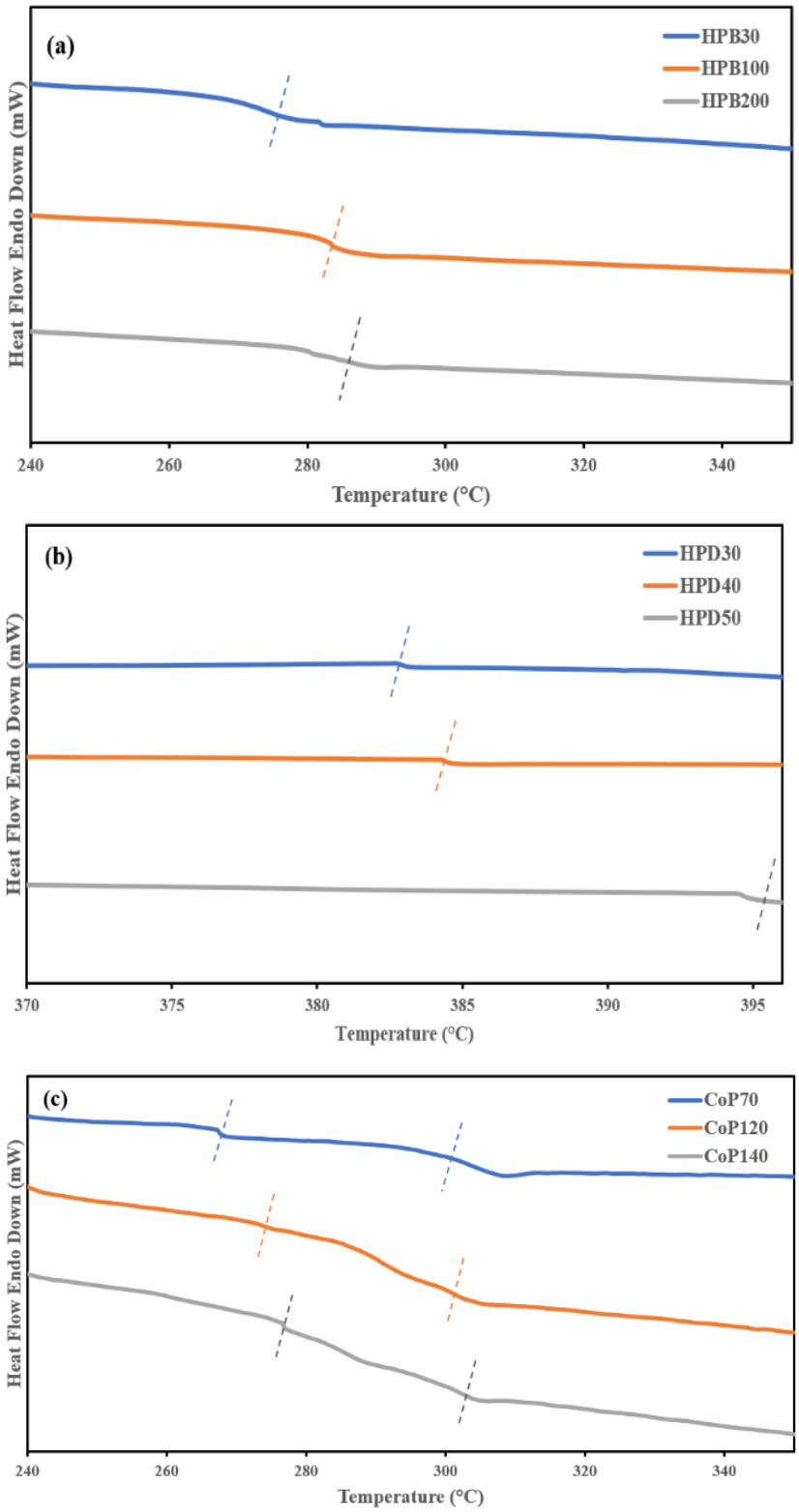


Figure S6. DSC thermograms of polyimide membranes with different Mw. (a) 6FDA-pBAPS, (b) 6FDA-DABA, and (c) 6FDA-pBAPS/DABA (3/1).

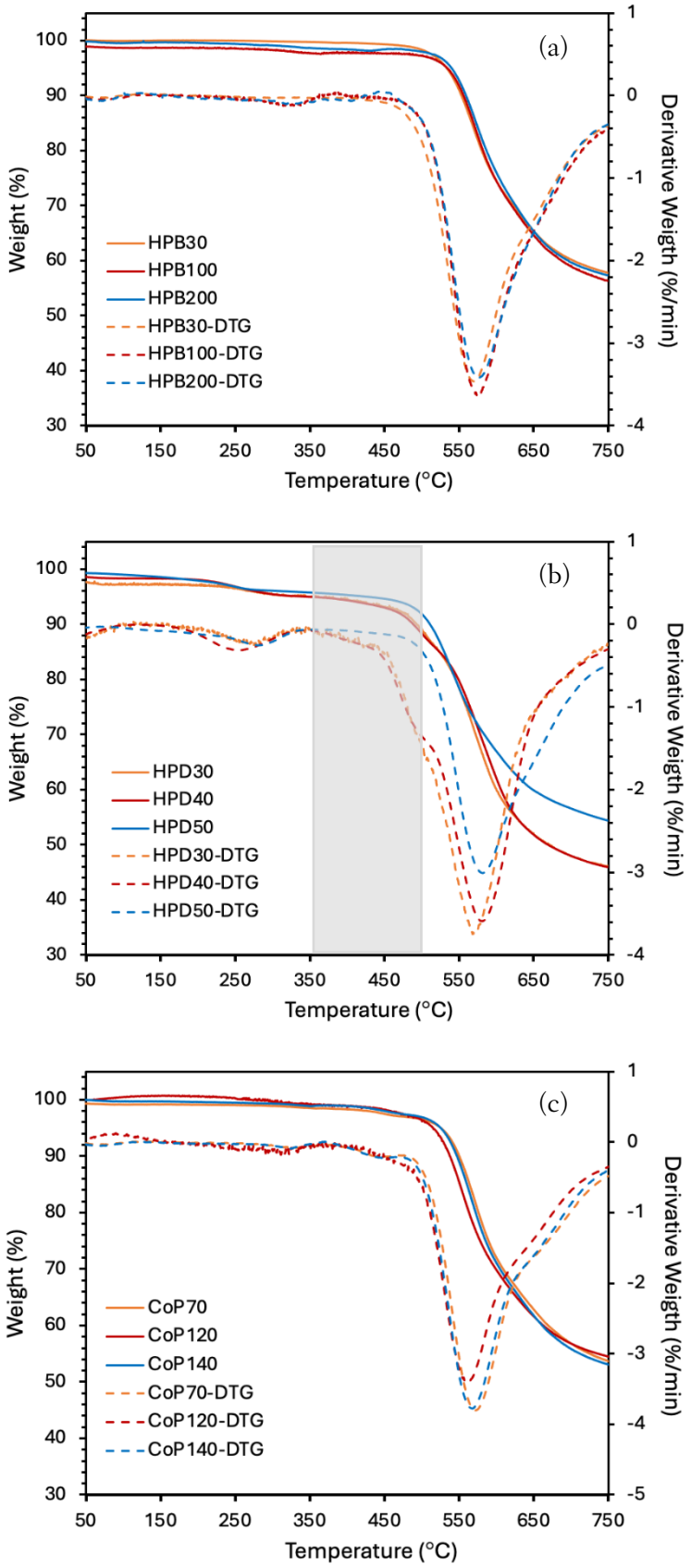


Figure S7. TGA/DTG thermograms of polyimide membranes with different M_w. (a) 6FDA-*p*BAPS, (b) 6FDA-DABA, and (c) 6FDA-*p*BAPS/DABA (3/1).

Table S2. Mechanical properties of polyimide membranes with different M_w.

Membrane	Tensile Strength (MPa)	Toughness (MJ/m^3)	Elongation at Break (%)
HPB30	82.174	3.91	7.94
HPB100	89.908	6.51	11.12
HPB200	91.707	11.38	15.59
HPD30	111.23	4.50	6.89
HPD40	107.98	4.16	6.62
HPD50	110.01	4.95	7.39
CoP70	91.132	3.72	6.89
CoP120	104.79	5.33	8.08
CoP140	115.51	8.26	10.8

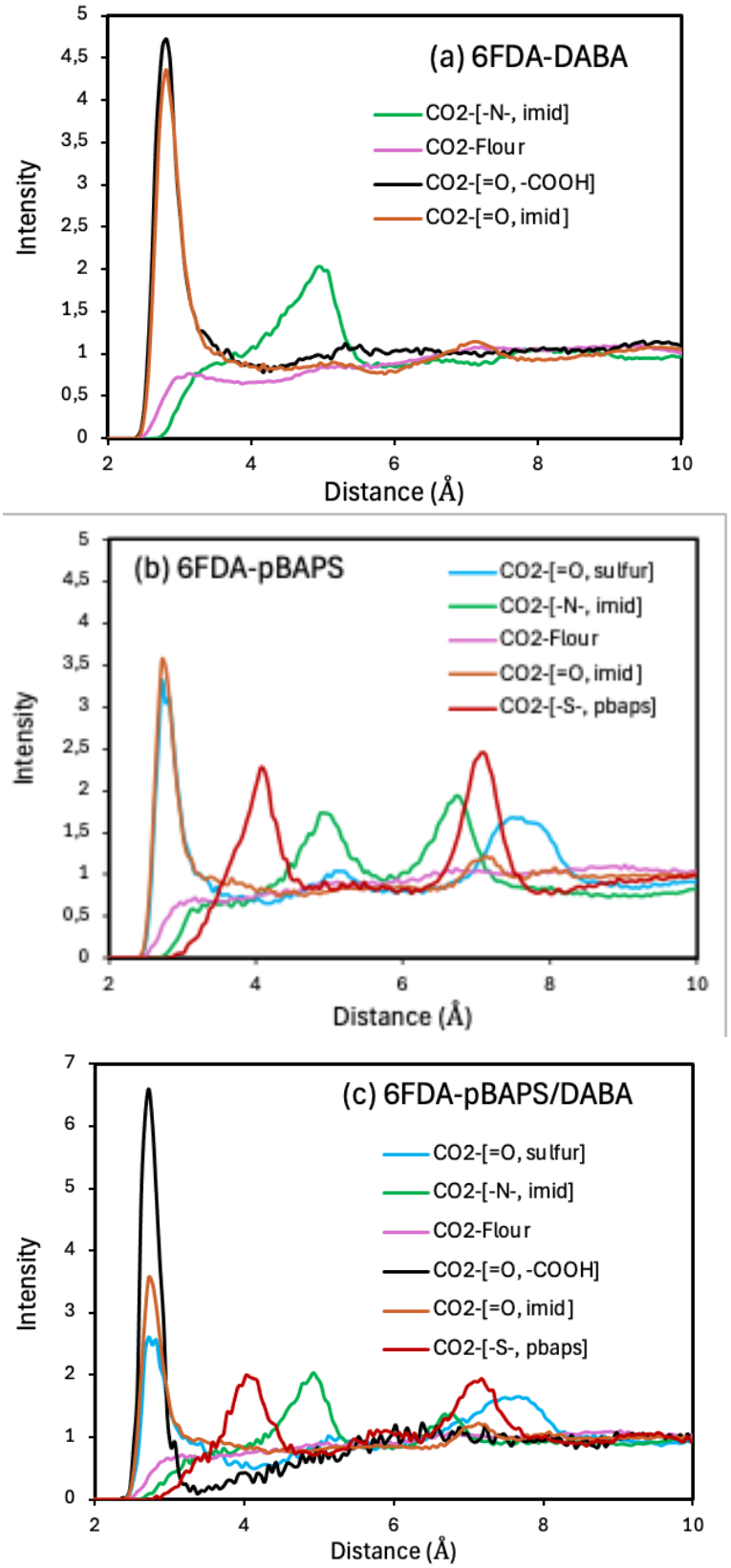


Figure S8. Radial distribution functions (RDFs) of the CO_2 molecule at 10 bar with the imide nitrogen (-N, imide), the carbonyl oxygen of the imide ring in the dianhydrides (=O, imide), the fluorine in the 6FDA dianhydride, the carboxylic acid oxygen (=O, -COOH) in the DABA diamine, the backbone oxygen (=O, sulfur) in the pBAPS diamine, and the sulfur linkage (-S-, pBAPS) for (a) 6FDA-DABA, (b) 6FDA-pBAPS, and (c) 6FDA-DABA/pBAPS polyimides.

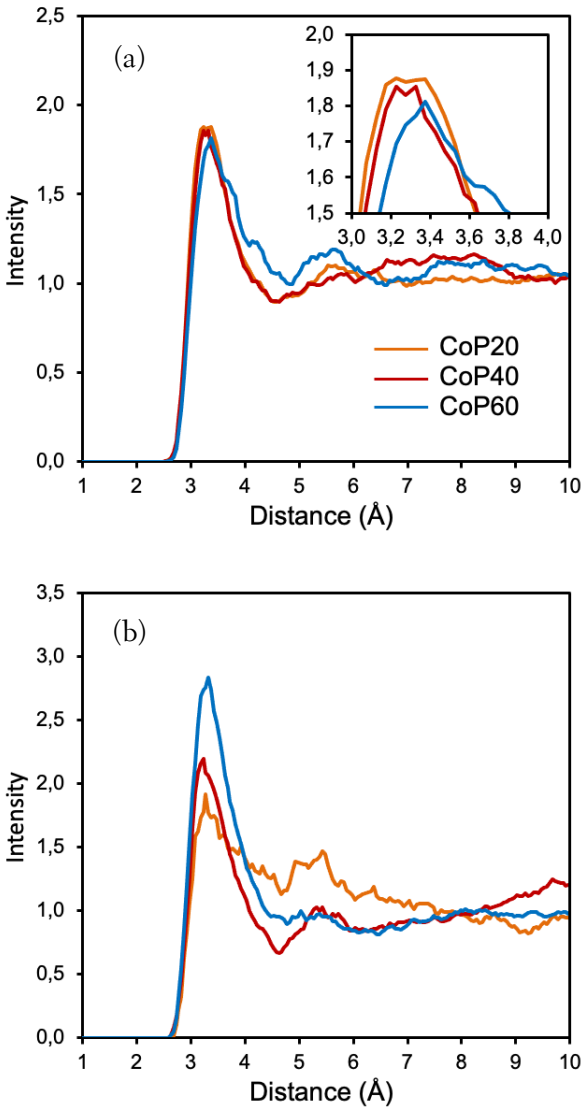


Figure S9. Radial distribution functions (RDFs) of the CO_2 molecule at 20 bar with (a) the sulfonyl backbone oxygen (=O, sulfur, O_3) in *p*BAPS, and (b) the carboxylic acid oxygen (=O, -COOH, O_2) in the DABA diamine for CoP.

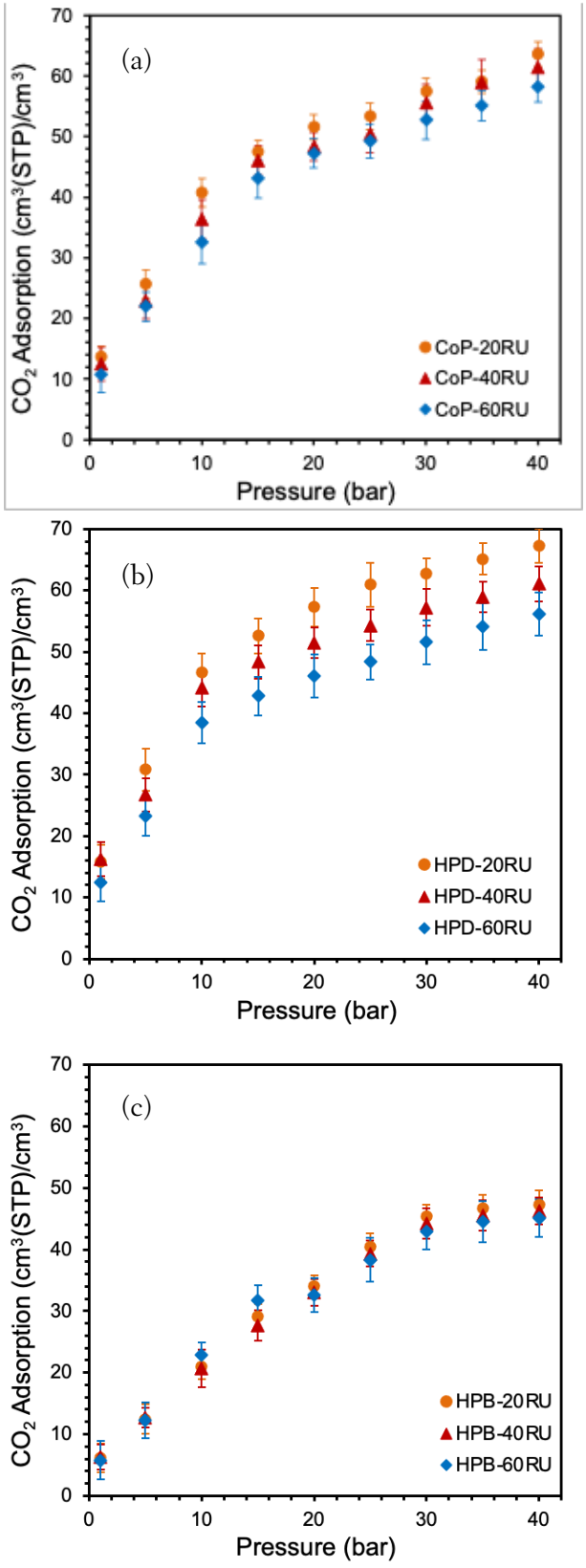


Figure S10. CO_2 sorption isotherm of (a) 6FDA-DABA/pBAPS, (b) 6FDA-DABA, and (c) 6FDA-pBAPS polyimides predicted from GCMC simulations up to 40 bar.