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Asymmetric thin-film mixed-matrix membranes with ZIF-8 in PVI-POEM comb copolymer achieving high CO_2 separation

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Jin Uk Kim[1], and Chang Soo Lee[*1]*

[1]Kumoh National Institute of Technology, Korea

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1. The title should be as brief as possible but long enough to indicate clearly the nature of the study. Capitalise the first letter of the first word ONLY (place names excluded). No full stop at the end.
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Numerous studies are underway on mixed-matrix membranes (MMMs) for gas separation, but it is still difficult to develop thin-film MMMs. In this study, a dual-functional imidazole-based comb copolymer and porous zeolitic imidazole framework (ZIF-8) were coated on poly(1-(trimethylsilyl)-1-propyne)/polysulfone (PTMSP/PSf) substrate *via* bar-coating method to fabricate a thin-film with high CO_2 permeance. The comb copolymer was poly(vinyl imidazole)-poly(oxyethylene methacrylate) (PVI-POEM) synthesized *via* free-radical polymerization, which indicated strong adhesion and good interaction between the filler and the matrix. In addition, the PVI-POEM-based MMMs showed in-situ formation of inverse asymmetric morphology and partial pore infiltration of PVI-POEM chains into ZIF-8 particles. Thus, the MMMs exhibited high CO_2 permeance without significant loss of selectivity at high ZIF-8 loading and low thickness. As a result, the 50 wt% ZIF-8 loading MMMs displayed optimal gas separation with CO_2 permeance of 4474 GPU and CO_2/N_2 and CO_2/CH_4 ideal selectivity of 32.0 and 12.4, respectively. The physiochemical interaction between PVI-POEM comb copolymer and ZIF-8 filler was investigated by analyzing the effects of morphological, structural, and energy characteristics on membrane performance through isothermal-isobaric molecular dynamics (NPT-MD) simulations.