Supplementary Information (SI) for Physical Chemistry Chemical Physics.
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Supplementary information for

Ionic Liquid-Mediated CO_2/N_2 Separation in $MoSe_2$ Nanochannels: A Molecular Dynamics Perspective

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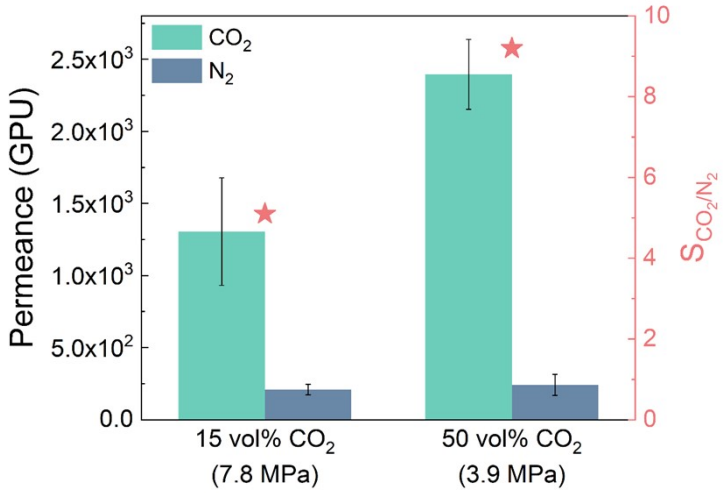

Figure S1 Permeance and selectivity of gases under different feed ratios and pressures.

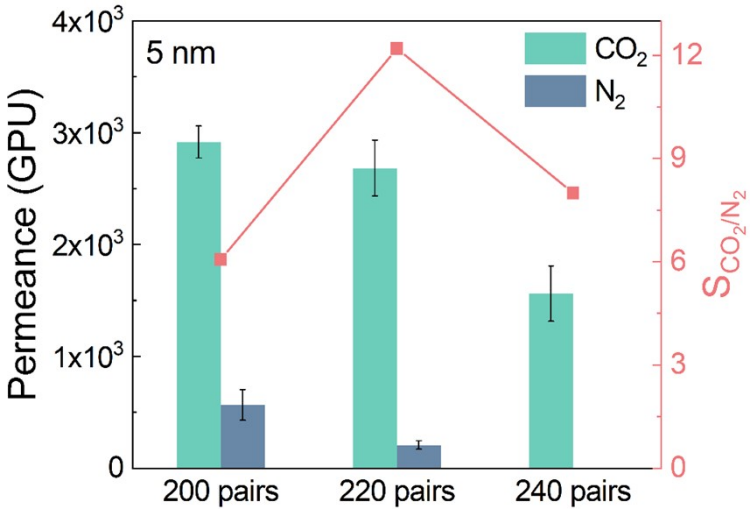

Figure S2 Gas permeance and separation selectivity at an interlayer spacing of 5 nm.

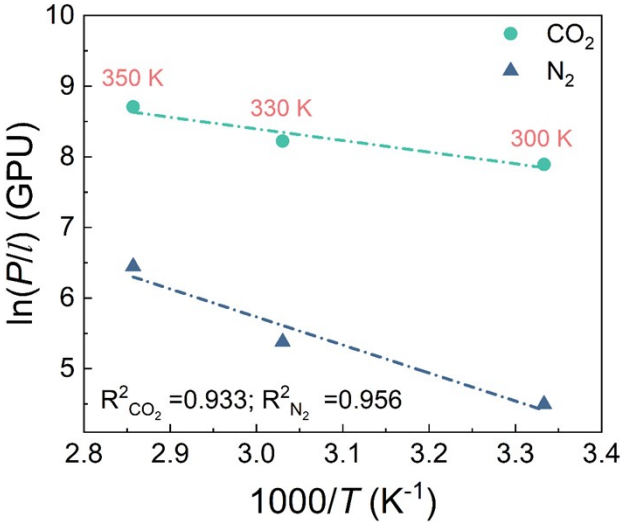

Figure S3 Arrhenius plots for gas permeance at an interlayer spacing of 4 nm.

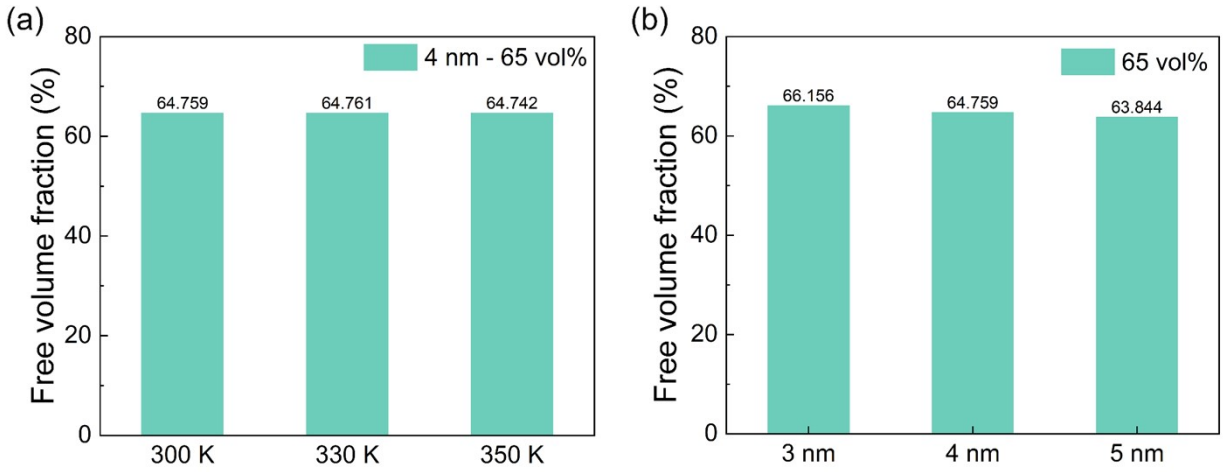

Figure S4 Free volume fraction within the nanochannel as a function of (a) temperature and (b) interlayer spacing.

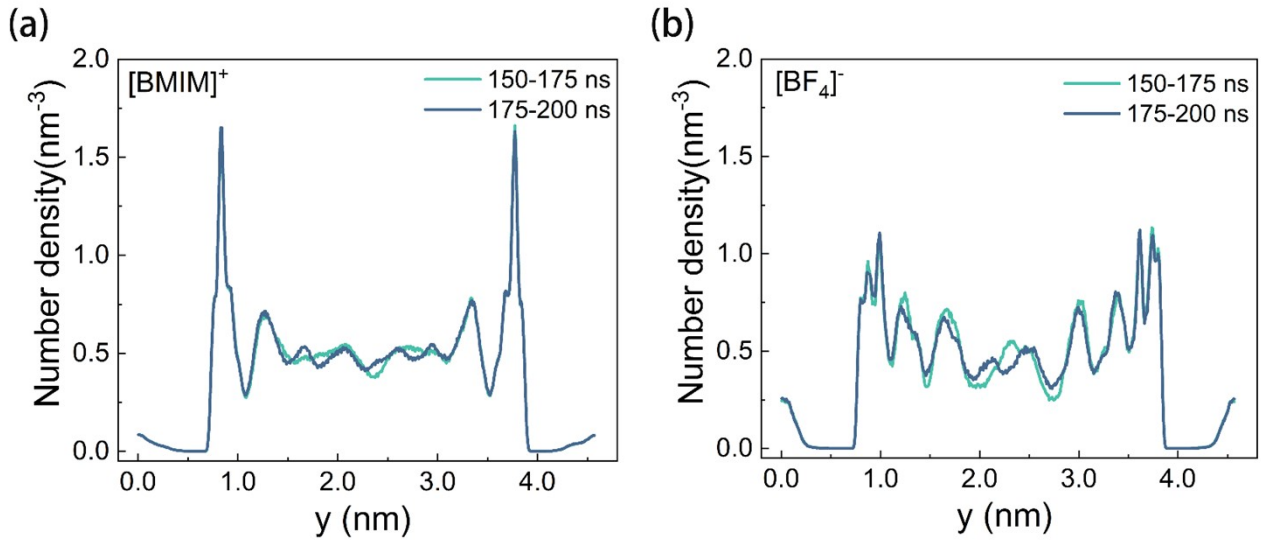

Figure S5 Number density distributions of (a) $[BMIM]^+$ and (b) $[BF_4]^-$ over two consecutive 25 ns intervals from the 150-200 ns simulation trajectory of the IL system.

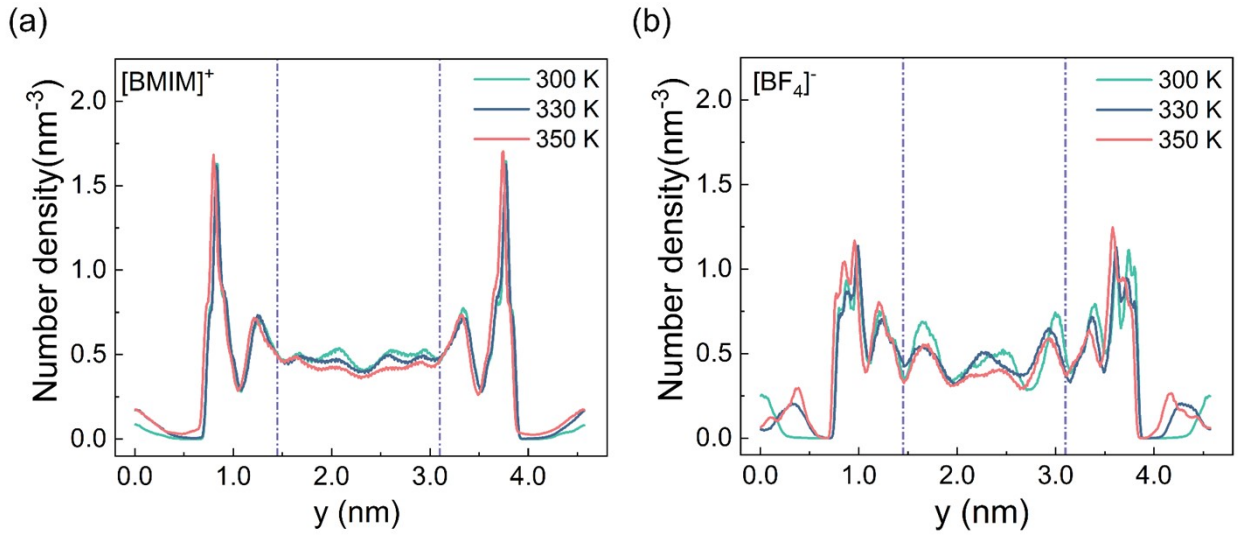

Figure S6 Number density distributions of (a) cations and (b) anions along the *y*-axis at different temperatures under a fixed interlayer spacing of 4 nm.

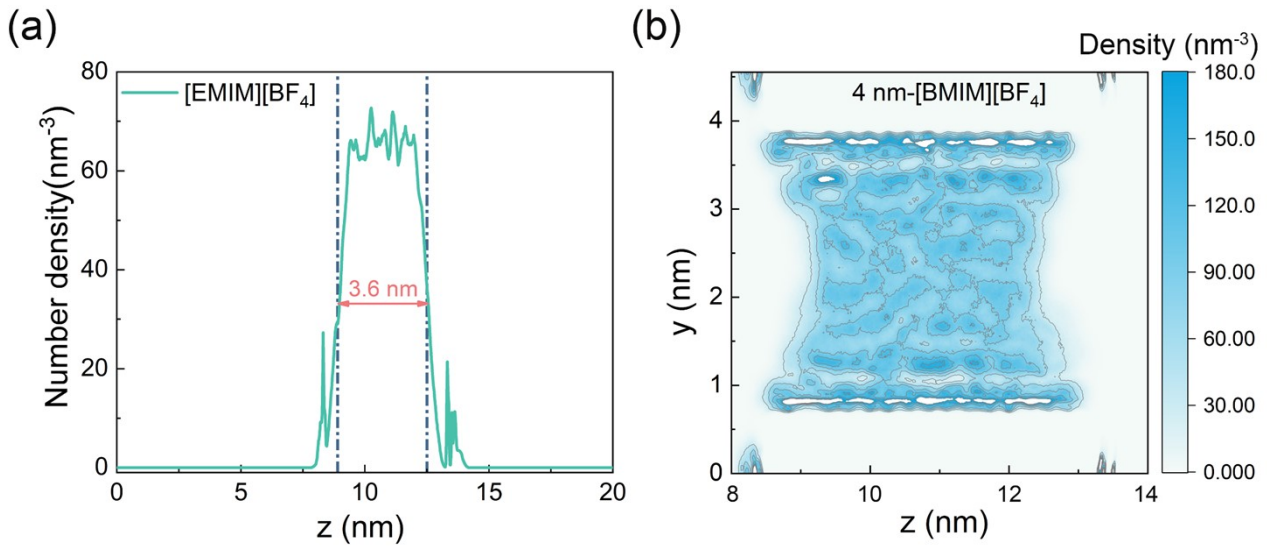

Figure S7 (a) Number density distribution of ILs along the *z*-axis and (b) the corresponding 2D density distribution at an interlayer spacing of 4 nm.

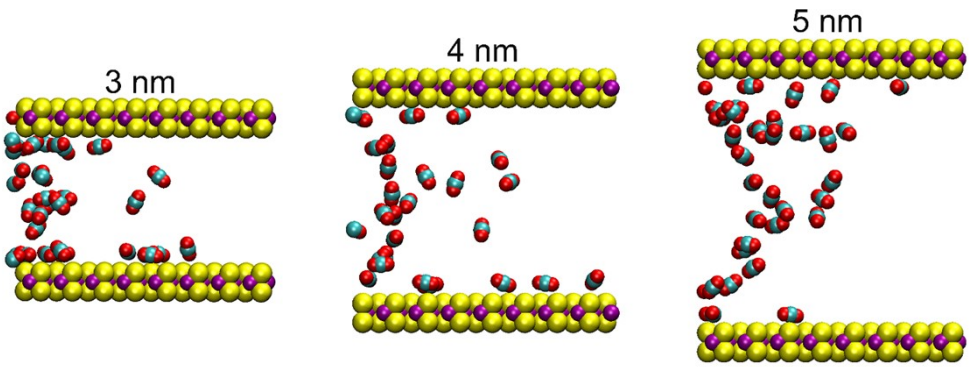

Figure S8 Snapshot illustrating the distribution of CO_2 within the nanochannels.

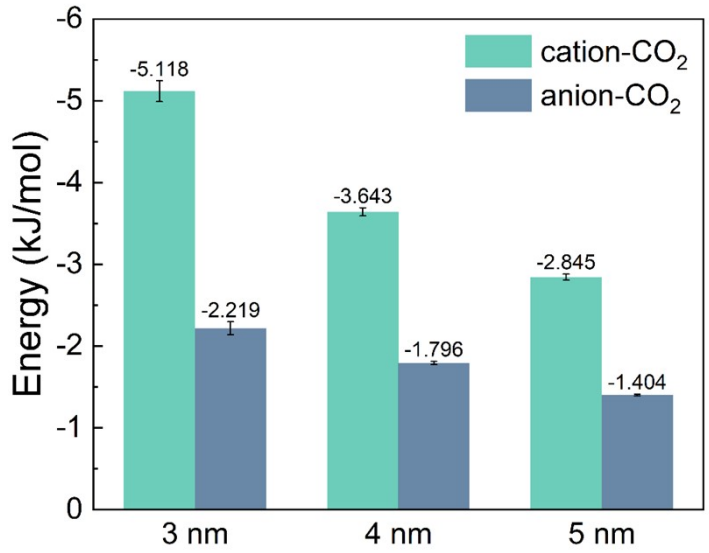

Figure S9 Interaction energy between CO_2 and cations/anions at different interlayer spacings.

Table S1 The permeability, diffusion coefficients, solubility coefficients, and corresponding selectivity of CO_2 and N_2 at three different layer spacings.

Interlayer spacing	Gas	Permeability (Barrer)	Diffusion coefficient (cm^2/s)	Solubility coefficient (cm^3 (STP*)/(cm^3·cmHg))
3 nm	CO_2	6.91	0.9168×10^{-5}	7.54×10^{-5}
	N_2	0.215	13.17×10^{-5}	1.63×10^{-7}
	selectivity	32.14	0.0696	462.58
4 nm	CO_2	9.61	4.446×10^{-5}	2.16×10^{-5}
	N_2	0.322	26.66×10^{-5}	1.21×10^{-7}
	selectivity	29.84	0.167	178.51
5 nm	CO_2	9.65	6.156×10^{-5}	1.57×10^{-5}
	N_2	0.752	37.86×10^{-5}	1.99×10^{-7}
	selectivity	12.83	0.163	78.89

*STP stands for standard temperature and pressure (0 °C, 1.0 atm).