

Supporting Information

Adsorptive process design for separation of hexane isomers using zeolites

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Figure S1. Computed adsorption isotherms of hexane isomers in MWW and MFI zeolites compared to available experimental data.¹⁻⁵

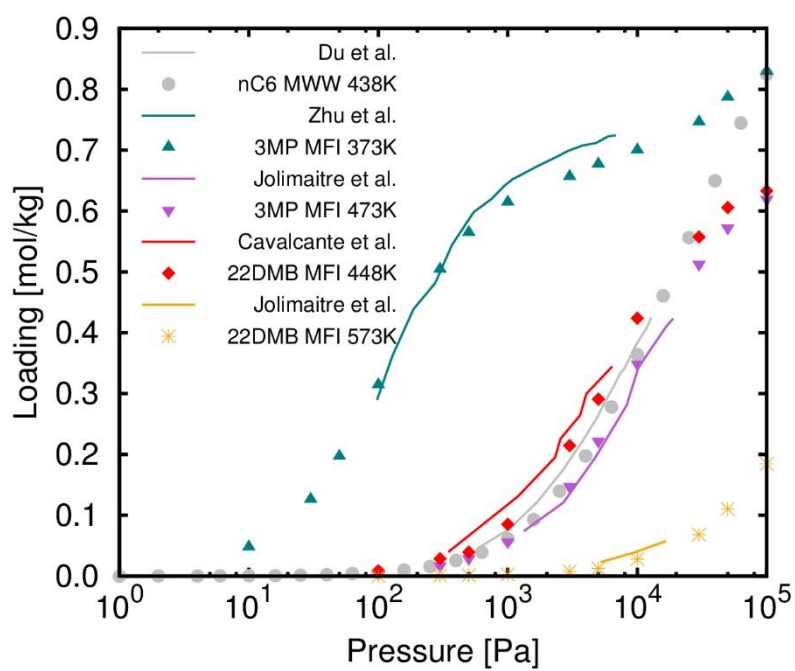


Table 1. Host-guest and guest-guest Lennard-Jones parameters used in this work. ϵ/K_B [K] in top row and $\sigma[\text{\AA}]$ in bottom row of each field.

	O	CH_4	CH_3	CH_2	CH	C
CH_4	115	158.5	130.84	94.21	51.91	11.26
	3.47	3.72	3.74	3.84	4.17	4.87
CH_3	93	130.84	108	77.77	42.85	9.3
	3.48	3.74	3.76	3.86	4.19	4.9
CH_2	60.5	94.21	77.77	56	30.85	6.69
	3.58	3.84	3.86	3.96	4.3	5.03
CH	40	51.91	42.85	30.85	17	3.69
	3.92	4.17	4.19	4.3	4.67	5.46
C	10	11.26	9.3	6.69	3.69	0.8
	4.56	4.87	4.9	5.03	5.46	6.38

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