Supplementary Information : Large-scale Computational Screening of Zeolites for Ethane/Ethene Separation

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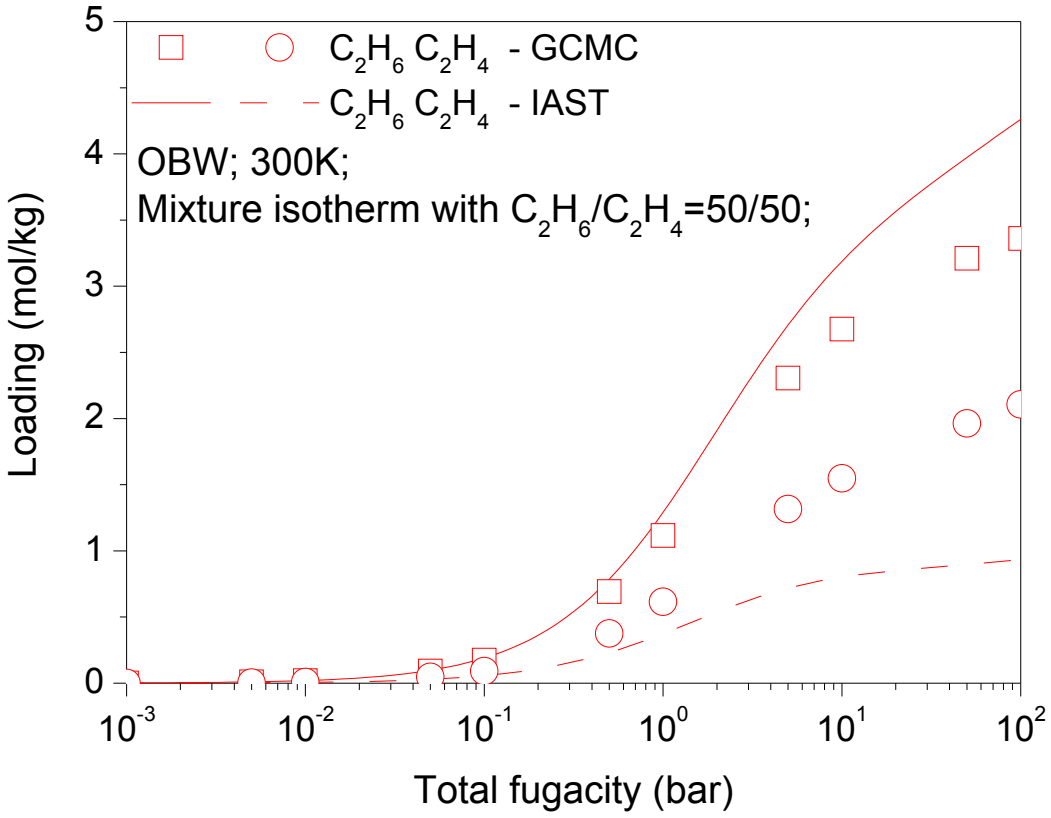

Figure SI 1: Comparison of the IAST-predicted mixture isotherm with GCMC-computed one in OBW. Open symbols show the GCMC-computed ethane-ethene (1:1) mixture isotherm in OBW at 300K as a function of total frugalities of the mixture. The lines show the predicted mixture isotherm by IAST.

Table SI 1: The Cartesian coordinates of the atoms of the preferential ethane binding geometry illustrated in Figure 7, from the framework of PCOD8156587. The coordinates are given with respect to the origin of the unit cell.

Atom	x(Å)	y(Å)	z(Å)
Si	9.000	10.889	7.793
Si	4.502	7.985	2.975
Si	9.000	7.985	6.661
Si	6.751	6.807	4.818
Si	2.250	7.136	4.818
Si	4.502	10.889	11.479
Si	6.751	12.066	9.636
Si	2.250	11.738	9.636
O	7.660	11.217	8.621
O	5.842	7.657	3.803
O	8.736	9.437	7.227
O	3.244	8.067	3.974
O	7.660	7.657	5.832
O	5.842	11.217	10.650
O	3.244	10.807	10.480