Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Supporting Information

C2 Adsorption in Zeolites: In Silico Screening and Sensitivity to Molecular Models

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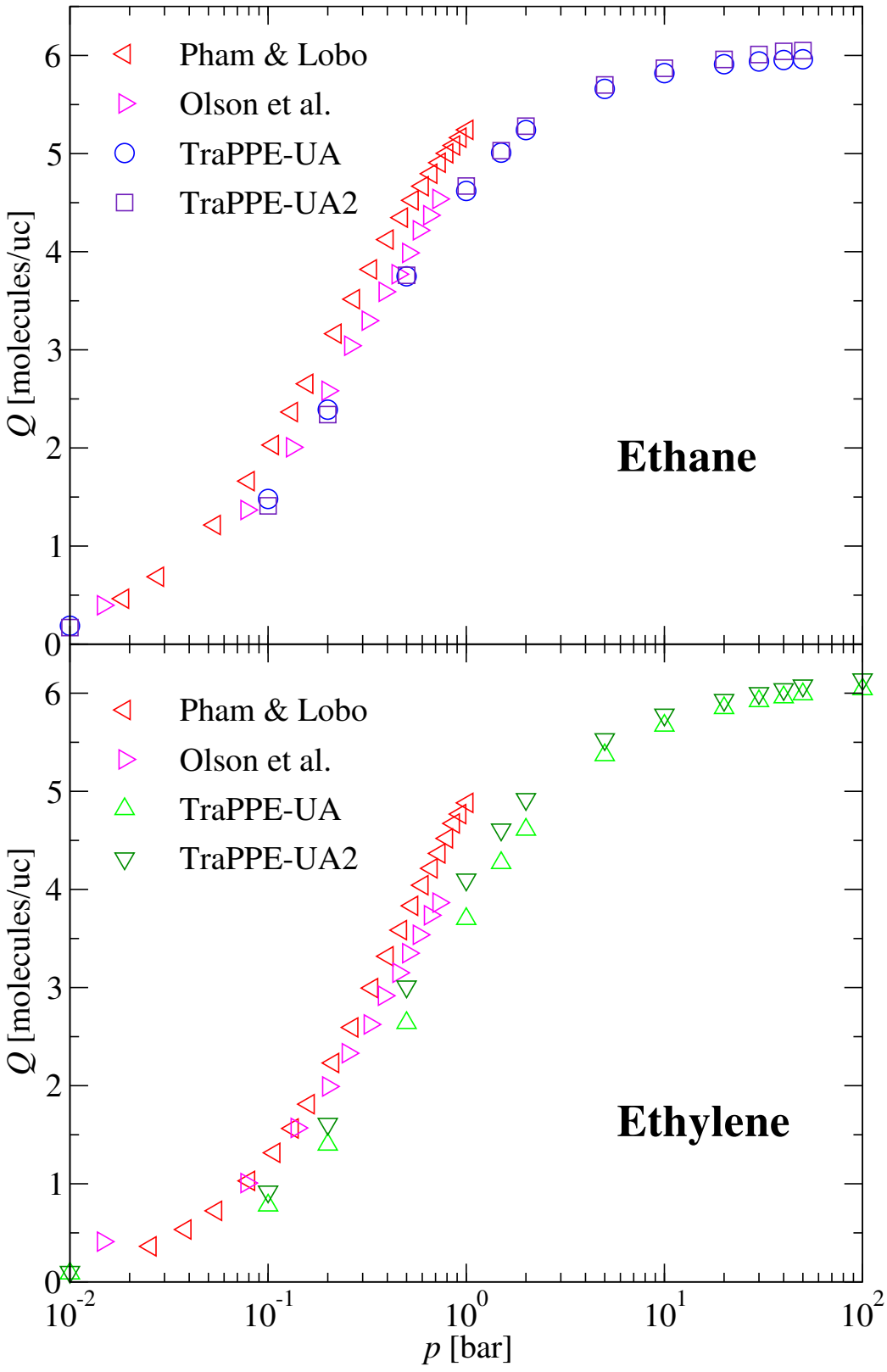

Figure S1: Unary adsorption isotherms of C_2H_6 (top) and C_2H_4 (bottom) at $T = 303$ K in CHA using the TraPPE–UA and TraPPE–UA2 models; experimental data are from Pham and Lobo[1] and Olson et al.[2]

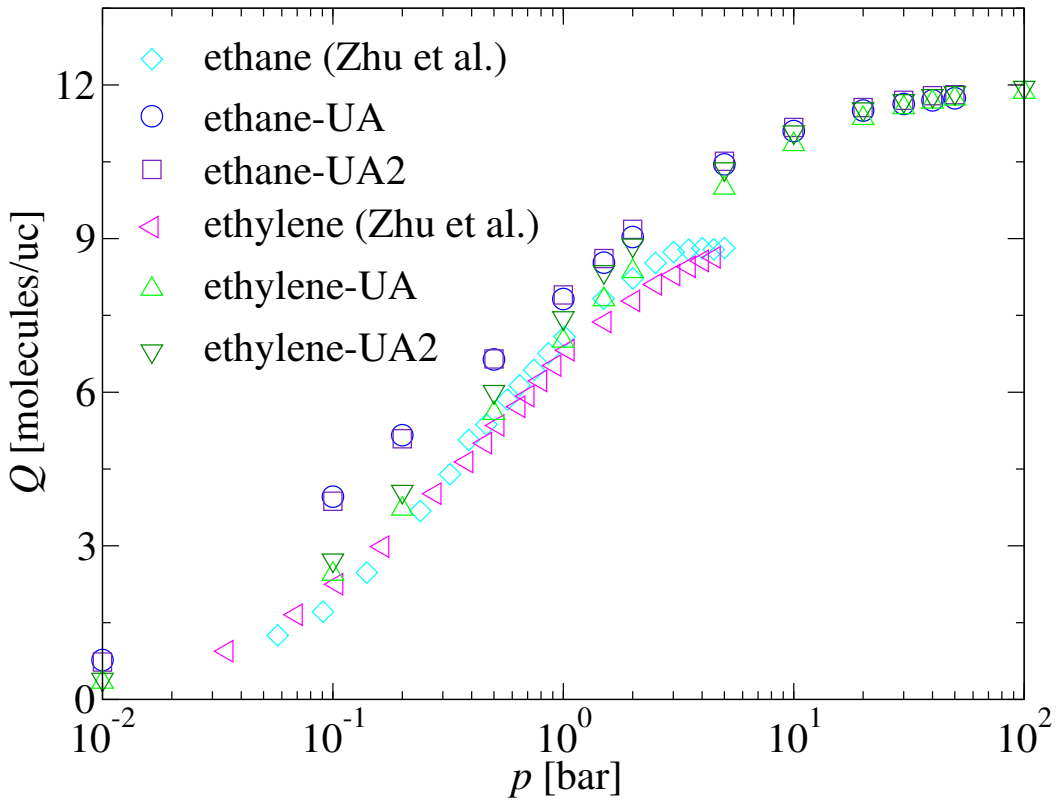

Figure S2: Unary adsorption isotherms of C_2H_4 and C_2H_6 at $T = 303$ K in DDR using various TraPPE models; experimental data are from Zhu et al.[3]

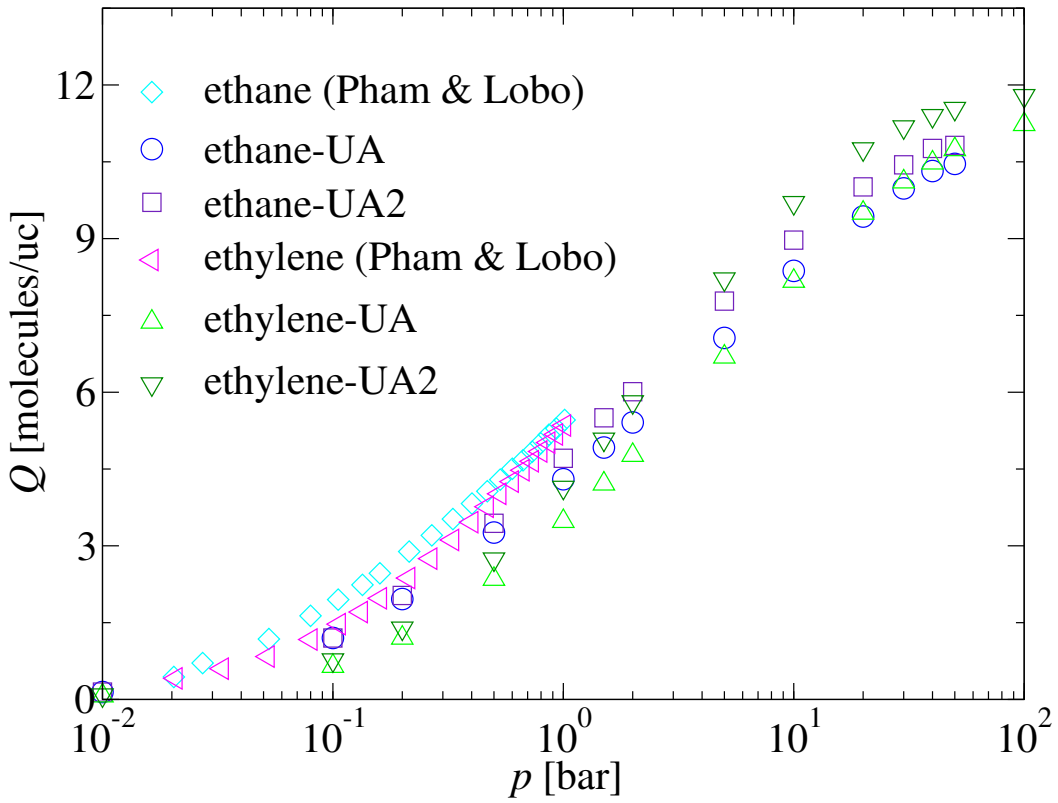

Figure S3: Unary adsorption isotherms of C_2H_4 and C_2H_6 at $T = 303$ K in AEI using various TraPPE models; experimental data are from Pham and Lobo.[1]

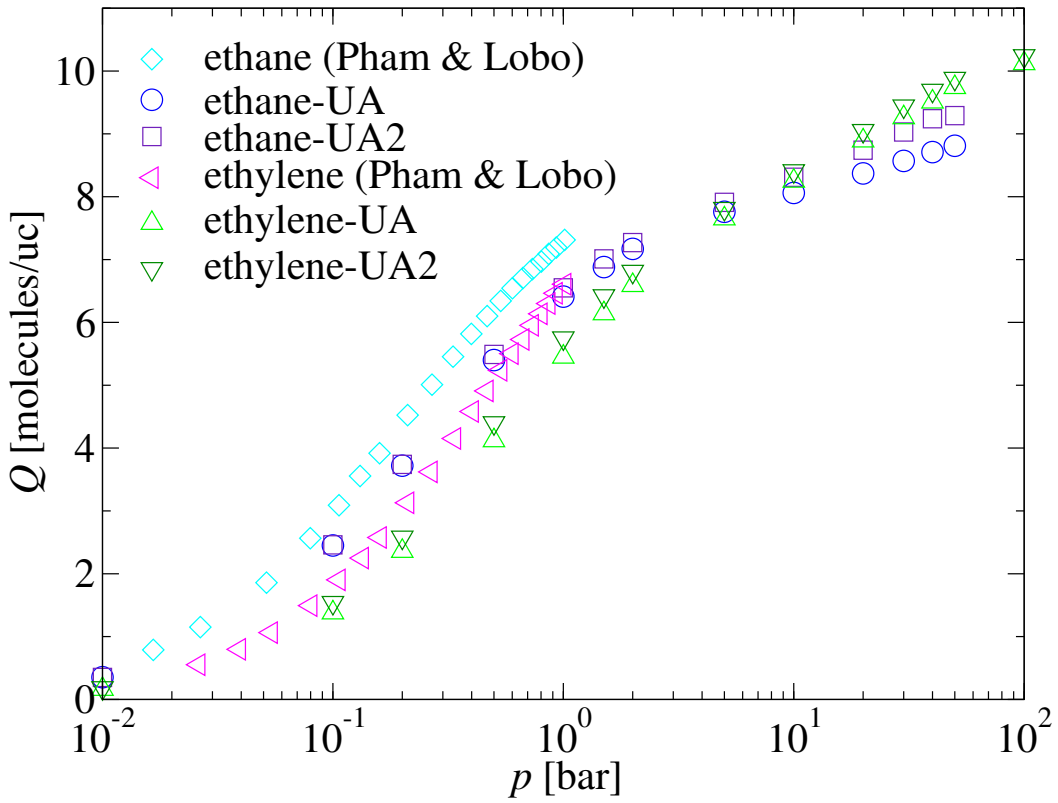

Figure S4: Unary adsorption isotherms of C_2H_4 and C_2H_6 at $T = 303$ K in STT using various TraPPE models; experimental data are from Pham and Lobo.[1]

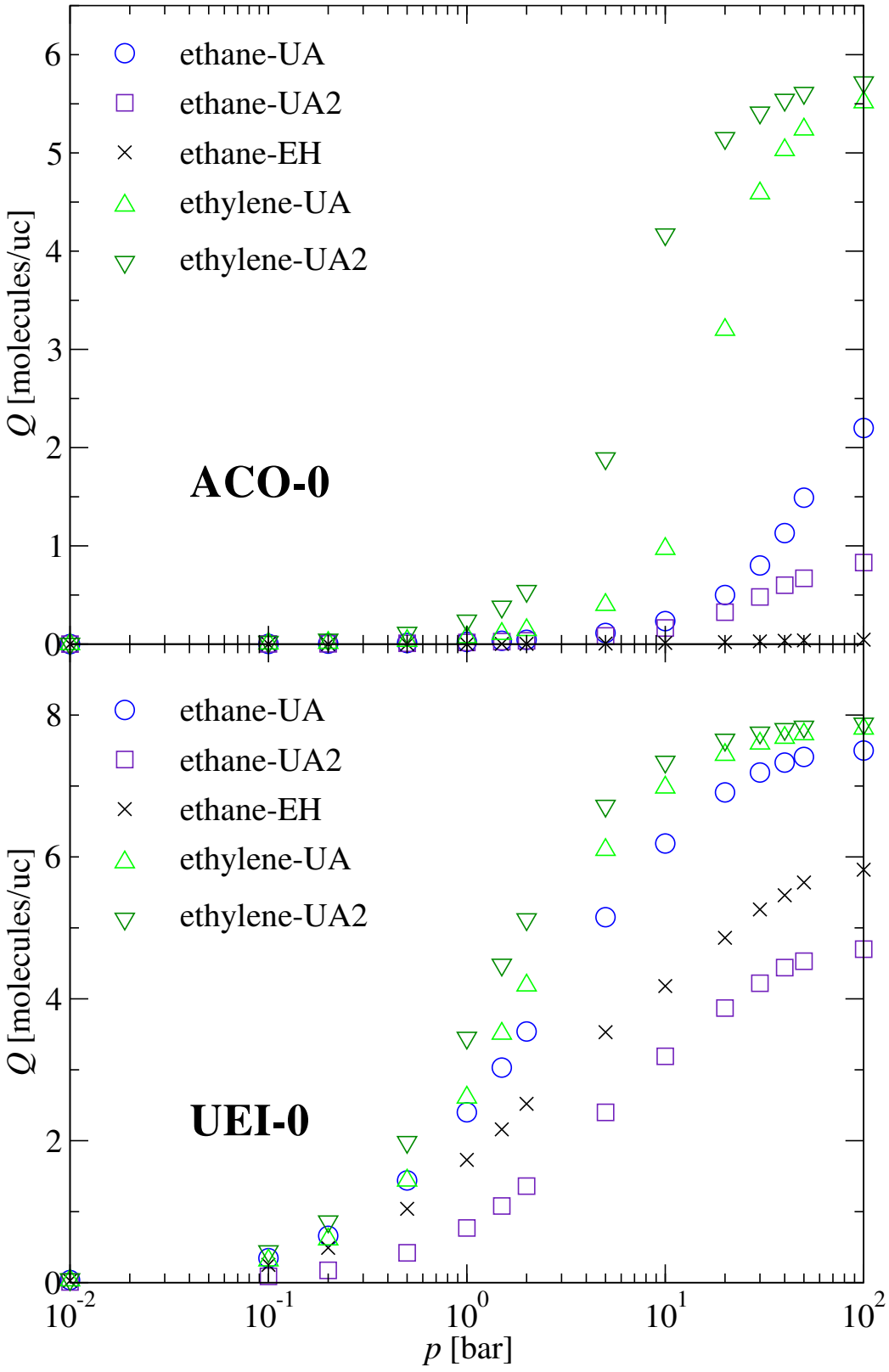

Figure S5: Unary adsorption isotherms of C_2H_4 and C_2H_6 at $T = 303$ K in ACO and UEI using various TraPPE models.

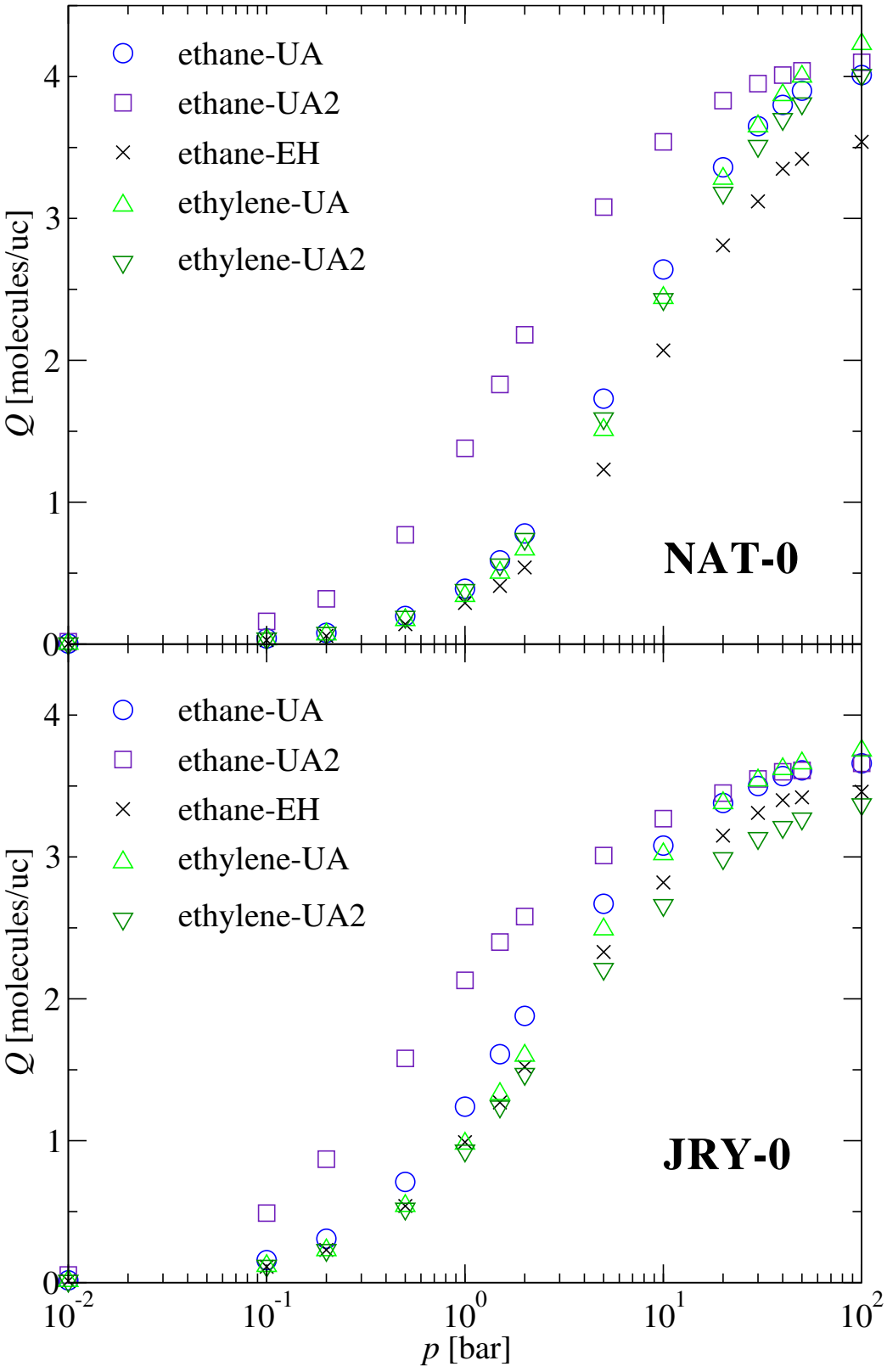

Figure S6: Unary adsorption isotherms of C_2H_4 and C_2H_6 at $T = 303$ K in NAT and JRY using various TraPPE models.

Table S1: Compositions, selectivities, and loadings [in mmol g^{-1}] in top-10 zeolites at $T = 300$ K, $p = 20$ bar, and $z_F = 0.5$.

zeolite	$x_{C_2H_4}$	$y_{C_2H_4}$	$S_{C_2H_4}$	$S_{C_2H_6}$	$Q_{C_2H_4}$	$Q_{C_2H_6}$
DFT	0.9599_2	0.3699_2	40.7_3	–	3.52	0.15
ACO	0.914_1	0.375_1	17.6_3	–	3.51	0.33
AWO	0.8824_4	0.4423_1	9.46_4	–	1.92	0.26
APD	0.838_1	0.4612_2	6.05_4	–	1.43	0.28
UEI	0.811_1	0.4426_2	5.41_4	–	2.10	0.49
SBN	0.719_3	0.4610_5	3.00_4	–	1.81	0.70
ITW	0.254_4	0.5318_5	–	3.3	0.48	1.42
NAT	0.257_2	0.5554_5	–	3.6	0.79	2.30
RRO	0.224_2	0.5251_2	–	3.8	0.31	1.08
JRY	0.215_1	0.5458_2	–	4.4	0.50	1.81

Subscript(s) indicate uncertainty in the last digit(s).

Table S2: Compositions, selectivities, and loadings [in mmol g^{-1}] in top-10 zeolites at $T = 300$ K, $p = 20$ bar, and $z_F = 0.9$.

zeolite	$x_{C_2H_4}$	$y_{C_2H_4}$	$S_{C_2H_4}$	$S_{C_2H_6}$	$Q_{C_2H_4}$	$Q_{C_2H_6}$
DFT	0.9967_2	0.8704_1	44_3	–	3.94	0.01
ACO	0.9931_1	0.85680_4	24.1_5	–	5.29	0.04
AWO	0.9862_4	0.8852_1	9.2_3	–	2.37	0.03
APD	0.978_1	0.8890_1	5.6_2	–	1.95	0.04
UEI	0.9708_5	0.8857_1	4.3_1	–	2.58	0.08
SBN	0.950_1	0.8883_2	2.39_5	–	2.99	0.16
ITW	0.783_3	0.9115_3	–	2.8	1.23	0.34
NAT	0.770_2	0.9267_5	–	3.8	2.19	0.65
RRO	0.730_5	0.9112_4	–	3.8	0.75	0.28
JRY	0.737_3	0.9242_5	–	4.4	1.58	0.57

Subscript(s) indicate uncertainty in the last digit(s).

Table S3: Compositions, selectivities, and loadings [in mmol g^{-1}] in top-10 zeolites at $T = 400$ K, $p = 50$ bar, and $z_F = 0.5$.

zeolite	$x_{C_2H_4}$	$y_{C_2H_4}$	$S_{C_2H_4}$	$S_{C_2H_6}$	$Q_{C_2H_4}$	$Q_{C_2H_6}$
DFT	0.949	0.471	21	–	0.97	0.053
ACO	0.877	0.489	7.4	–	0.40	0.056
AWO	0.893	0.481	9.0	–	0.69	0.083
APD	0.843	0.489	5.6	–	0.44	0.082
UEI	0.783	0.476	4.0	–	1.0	0.28
SBN	0.733	0.492	2.8	–	0.40	0.15
ITW	0.389	0.508	–	1.6	0.44	0.69
NAT	0.312	0.519	–	2.4	0.46	1.0
RRO	0.306	0.506	–	2.3	0.15	0.34
JRY	0.302	0.519	–	2.5	0.45	1.0

Subscript(s) indicate uncertainty in the last digit(s).

Table S4: Compositions, selectivities, loadings [in mmol g^{-1}], and performance criteria [in mmol g^{-1}] for all zeolites from the IZA database used in the screening study using the TraPPE–UA2 force field at $T = 300$ K, $p = 20$ bar, and $z_F = 0.5$. Subscript(s) indicate uncertainty in the last digit(s). "n.d." indicates "not defined". Asterisk after the framework type in the first column indicates that the largest pore window for this framework, obtained from the IZA–SC database,[4] is 3.4 Å. The idealized all-silica zeolite topologies are represented as XXX, while XXX-i ($i = 1, 2, ...$) corresponds to an experimental structure.

zeolite	$x_{C_2H_4}$	$y_{C_2H_4}$	$S_{C_2H_4}$	$S_{C_2H_6}$	$Q_{C_2H_4}$	$Q_{C_2H_6}$	P
ABW	0.0177_1	0.50498_5	0.0176_1	56.7_3	0.0030	0.17	0.67
ACO	0.914_1	0.375_1	17.6_3	0.057_1	3.5	0.33	10
AEI	0.468_2	0.509_1	0.85_1	1.18_1	1.7	1.9	0.31
AEL	0.312_2	0.5184_2	0.422_4	2.37_2	0.46	1.0	0.88
AEN	0.094_1	0.5099_1	0.100_1	10.0_1	0.037	0.36	0.83
AET	0.395_1	0.5111_1	0.624_4	1.60_1	0.63	0.96	0.45
AFG*	0.469_3	0.5041_3	0.87_1	1.15_1	0.92	1.0	0.15
AFI	0.381_4	0.5160_5	0.58_1	1.73_3	0.76	1.2	0.67
AFN*	0.353_3	0.5144_4	0.52_1	1.94_3	0.52	0.96	0.64
AFO	0.314_2	0.5190_3	0.425_5	2.35_3	0.48	1.1	0.91
AFR	0.458_5	0.511_1	0.81_2	1.24_3	1.6	1.9	0.41
AFS	0.491_3	0.503_1	0.95_1	1.05_2	1.9	1.9	0.094
AFT	0.417_2	0.5178_4	0.67_1	1.50_1	1.2	1.7	0.70
AFX-1	0.544_2	0.4903_4	1.24_1	0.81_1	1.6	1.4	0.35
AFY	0.484_1	0.508_1	0.91_1	1.10_1	2.7	2.8	0.28
AHT*	0.033_1	0.5	0.034_1	29_1	0.000087	0.0012	0.0040
ANA*	0	0.5	0	n.d.	0	0	n.d.
APC*	0.705_4	0.49877_3	2.40_5	0.42_1	0.070	0.030	0.062
APD	0.838_1	0.4612_2	6.05_4	0.165_1	1.4	0.28	2.6
AST*	0.377_1	0.5240_3	0.550_3	1.82_1	1.0	1.7	1.0

ASV	0.663_3	0.4821_3	2.11_3	0.47_1	1.1	0.56	0.82
ATN	0.613_2	0.4840_3	1.69_2	0.59_1	1.3	0.80	0.66
ATO	0.530_4	0.4975_3	1.14_2	0.88_2	0.68	0.60	0.089
ATS	0.413_2	0.5162_4	0.66_1	1.52_2	1.1	1.5	0.64
ATT	0.626_4	0.475_1	1.85_4	0.54_1	1.7	1.0	1.1
ATV	0.902_1	0.4783_1	10.0_2	0.100_2	0.77	0.083	1.8
AWO	0.8824_4	0.4423_1	9.46_4	0.1057_4	1.9	0.26	4.3
AWW	0.351_3	0.5168_4	0.51_1	1.98_3	0.59	1.1	0.74
BCT*	0	0.5	0	n.d.	0	0	n.d.
BEA	0.438_2	0.5147_5	0.74_1	1.36_1	1.4	1.8	0.55
BEC	0.403_3	0.523_1	0.62_1	1.62_3	1.3	1.9	0.91
BIK	0.0091_2	0.5055_1	0.0090_2	111_3	0.0017	0.18	0.85
BOF	0.553_4	0.490_1	1.29_3	0.78_2	1.4	1.1	0.36
BOG	0.413_3	0.518_1	0.65_1	1.53_2	1.2	1.7	0.72
BOZ	0.440_1	0.5183_3	0.729_4	1.37_1	1.7	2.2	0.69
BPH	0.456_4	0.511_1	0.80_2	1.25_2	1.5	1.8	0.41
BRE*	0.488_3	0.5017_4	0.95_1	1.06_1	1.0	1.1	0.059
BSV	0.590_3	0.4837_5	1.53_2	0.65_1	1.5	1.0	0.65
CAN	0.442_2	0.5055_2	0.78_1	1.29_1	0.64	0.80	0.20
CAS*	0.99734_5	0.4820_1	402_8	0.00249_5	0.58	0.0015	3.5
CDO	0.523_4	0.4972_4	1.11_2	0.90_1	0.96	0.87	0.099
CFI	0.369_3	0.5148_4	0.55_1	1.81_3	0.63	1.1	0.63
CGF*	0.526_4	0.4968_5	1.12_2	0.89_2	0.96	0.87	0.11
CGS	0.420_3	0.5113_4	0.69_1	1.44_2	0.87	1.2	0.44
CON	0.410_4	0.519_1	0.64_1	1.56_3	1.2	1.7	0.77
CSV	0.411_4	0.520_1	0.64_1	1.55_3	1.2	1.8	0.77
CZP	0.096_1	0.5168_1	0.099_2	10.1_2	0.064	0.60	1.4

DAC	0.653_{1}	0.4681_{1}	2.14_{1}	0.468_{2}	1.9	1.0	1.4
DDR	0.533_{3}	0.4955_{4}	1.16_{1}	0.86_{1}	1.1	0.92	0.16
DFO	0.435_{3}	0.518_{1}	0.72_{1}	1.40_{2}	1.5	2.0	0.67
DFT	0.9599_{2}	0.3699_{2}	40.7_{3}	0.0245_{2}	3.5	0.15	13
DOH*	0.716_{2}	0.444_{1}	3.17_{4}	0.316_{4}	2.5	0.98	2.8
DON	0.406_{4}	0.5129_{5}	0.65_{1}	1.54_{3}	0.82	1.2	0.52
EAB	0.421_{4}	0.516_{1}	0.68_{1}	1.46_{3}	1.2	1.6	0.60
EDI	0.647_{1}	0.4640_{3}	2.11_{1}	0.473_{3}	2.1	1.2	1.6
EEI*	0.365_{3}	0.5117_{2}	0.55_{1}	1.83_{2}	0.48	0.84	0.51
EMT	0.496_{2}	0.502_{1}	0.98_{1}	1.02_{1}	2.4	2.4	0.055
EON	0.539_{4}	0.494_{1}	1.20_{2}	0.84_{2}	1.2	1.0	0.21
EPI	0.574_{3}	0.4854_{5}	1.43_{2}	0.70_{1}	1.6	1.2	0.56
ERI	0.422_{4}	0.515_{1}	0.69_{1}	1.46_{3}	1.1	1.5	0.57
ESV	0.362_{5}	0.5127_{5}	0.54_{1}	1.85_{4}	0.51	0.89	0.55
ETL	0.381_{4}	0.5069_{2}	0.60_{1}	1.67_{3}	0.35	0.57	0.29
ETR	0.410_{5}	0.518_{1}	0.65_{2}	1.55_{4}	1.1	1.6	0.71
EUO	0.359_{2}	0.5184_{3}	0.52_{1}	1.92_{2}	0.69	1.2	0.81
EWS	0.425_{2}	0.5117_{3}	0.71_{1}	1.42_{1}	0.95	1.3	0.45
EZT	0.501_{4}	0.500_{1}	1.00_{2}	1.00_{2}	1.2	1.2	0.0038
FAR*	0.472_{4}	0.505_{1}	0.88_{2}	1.14_{2}	1.1	1.2	0.16
FAU	0.498_{2}	0.501_{1}	0.99_{1}	1.01_{1}	2.4	2.5	0.029
FER	0.483_{4}	0.503_{1}	0.92_{2}	1.08_{2}	1.1	1.1	0.089
FRA*	0.430_{3}	0.514_{1}	0.71_{1}	1.40_{2}	1.2	1.5	0.52
GIS*	0.484_{3}	0.505_{1}	0.92_{1}	1.09_{2}	1.8	2.0	0.16
GIU*	0.45_{1}	0.506_{1}	0.81_{2}	1.24_{3}	0.89	1.1	0.23
GME	0.430_{1}	0.5172_{2}	0.704_{3}	1.42_{1}	1.4	1.9	0.66
GON	0.377_{3}	0.5091_{3}	0.58_{1}	1.71_{3}	0.43	0.72	0.39

GOO*	0.327_{2}	0.5201_{3}	0.448_{5}	2.23_{2}	0.57	1.2	0.94
HEU	0.654_{2}	0.4715_{4}	2.11_{2}	0.473_{5}	1.7	0.90	1.3
IFO	0.371_{5}	0.518_{1}	0.55_{1}	1.82_{4}	0.75	1.3	0.76
IFR	0.372_{4}	0.5190_{5}	0.55_{1}	1.82_{3}	0.80	1.3	0.81
IFU	0.396	0.593	0.449	2.2	0.46	0.69	0.55
IFW	0.464_{1}	0.5080_{3}	0.84_{1}	1.19_{1}	1.4	1.6	0.29
IFY	0.442_{2}	0.5087_{4}	0.77_{1}	1.31_{2}	0.96	1.2	0.32
IHW	0.399_{3}	0.5107_{3}	0.64_{1}	1.57_{2}	0.64	0.96	0.43
IMF	0.48_{1}	0.504_{1}	0.90_{2}	1.11_{3}	1.1	1.2	0.12
IRN	0.432_{2}	0.5154_{4}	0.72_{1}	1.40_{1}	1.3	1.8	0.58
IRR	0.448_{3}	0.525_{1}	0.73_{1}	1.36_{2}	2.4	3.0	0.93
ISV	0.413_{1}	0.5207_{3}	0.649_{4}	1.54_{1}	1.3	1.9	0.82
ITE	0.479_{3}	0.505_{1}	0.90_{1}	1.11_{2}	1.5	1.6	0.17
ITG	0.401_{2}	0.5160_{3}	0.63_{1}	1.59_{1}	0.93	1.4	0.65
ITH	0.445_{2}	0.5074_{3}	0.78_{1}	1.28_{1}	0.87	1.1	0.27
ITR	0.455_{4}	0.5056_{5}	0.82_{1}	1.23_{2}	0.84	1.0	0.20
ITT	0.480_{3}	0.509_{1}	0.89_{2}	1.12_{2}	2.4	2.6	0.30
ITW	0.254_{4}	0.5318_{5}	0.30_{1}	3.3_{1}	0.48	1.4	1.7
ITW-1	0.547	0.452	1.466	0.68	0.76	0.63	0.29
IWR	0.406_{3}	0.520_{1}	0.63_{1}	1.59_{2}	1.2	1.8	0.81
IWS	0.408_{2}	0.5226_{5}	0.63_{1}	1.59_{2}	1.3	1.9	0.90
IWV	0.441_{1}	0.5157_{2}	0.741_{3}	1.35_{1}	1.5	2.0	0.58
IWW	0.428_{5}	0.512_{1}	0.71_{2}	1.40_{3}	1.0	1.4	0.46
JBW	0.0129_{1}	0.5170_{1}	0.0122_{1}	82_{1}	0.0073	0.55	2.4
JNT*	0.256_{2}	0.5148_{1}	0.324_{3}	3.09_{3}	0.24	0.71	0.80
JOZ	0.416_{2}	0.5174_{4}	0.66_{1}	1.51_{2}	1.2	1.7	0.68
JRY	0.215_{1}	0.5458_{2}	0.228_{2}	4.38_{4}	0.50	1.8	2.7

JSN	0.350_4	0.521_1	0.49_1	2.02_4	0.73	1.4	0.95
JSR	0.438_4	0.531_2	0.69_2	1.46_4	2.4	3.1	1.2
JST	0.493_4	0.502_1	0.96_2	1.04_2	1.9	2.0	0.073
JSW*	0.325_4	0.5158_4	0.45_1	2.22_4	0.45	0.93	0.74
KFI	0.403_2	0.5199_5	0.62_1	1.61_2	1.1	1.7	0.80
LAU	0.520_4	0.4970_5	1.10_2	0.91_2	1.1	1.0	0.10
LEV	0.383_3	0.5173_5	0.58_1	1.73_3	0.82	1.3	0.72
LIO*	0.487_4	0.5014_4	0.94_2	1.06_2	0.83	0.88	0.050
LOS*	0.473_2	0.5048_4	0.88_1	1.14_1	1.2	1.3	0.17
LOV	0.685_1	0.4656_2	2.49_1	0.401_2	1.8	0.83	1.6
LTA	0.466_4	0.511_1	0.83_2	1.20_3	2.0	2.3	0.41
LTF	0.437_3	0.5076_4	0.75_1	1.33_2	0.78	1.0	0.28
LTJ*	0.64_2	0.5	1.7_1	0.57_4	0.0023	0	0.0013
LTL	0.449_2	0.5078_4	0.79_1	1.27_1	0.99	1.2	0.29
LTN*	0.481_5	0.503_1	0.91_2	1.09_2	1.1	1.2	0.11
MAR*	0.508_4	0.499_1	1.04_2	0.97_2	0.99	0.96	0.035
MAZ	0.413_5	0.512_1	0.67_1	1.49_3	0.81	1.2	0.46
MEI	0.440_2	0.5176_5	0.73_1	1.36_1	1.7	2.1	0.66
MEL	0.478_2	0.5036_3	0.90_1	1.11_1	1.1	1.2	0.12
MEP*	0.492_2	0.5017_4	0.96_1	1.04_1	1.4	1.4	0.057
MER	0.621_2	0.4807_3	1.77_2	0.56_1	1.4	0.87	0.81
MFI	0.412_2	0.5125_3	0.67_1	1.50_2	0.86	1.2	0.49
MFS	0.456_5	0.505_1	0.82_2	1.22_3	0.82	0.98	0.20
MON	0.0161_2	0.5075_1	0.0159_2	63_1	0.0040	0.25	1.0
MOR	0.660_2	0.4692_4	2.19_2	0.456_5	1.8	0.91	1.4
MOZ	0.488_2	0.5018_3	0.95_1	1.06_1	1.0	1.1	0.061
MRE	0.461_3	0.5033_2	0.84_1	1.18_1	0.59	0.69	0.12

MSE	0.405_3	0.516_1	0.64_1	1.57_3	0.98	1.4	0.64
MSO*	0.410_3	0.5103_4	0.67_1	1.50_2	0.70	1.0	0.41
MTN*	0.723_1	0.4526_2	3.15_1	0.317_1	2.1	0.81	2.4
MTT	0.368_5	0.5118_4	0.56_1	1.80_4	0.50	0.87	0.51
MTW	0.366_4	0.5111_3	0.55_1	1.81_3	0.47	0.81	0.48
MVY*	0	0.5	0	n.d.	0	0	n.d.
MWW	0.442_5	0.513_1	0.75_2	1.33_4	1.3	1.7	0.48
NAB	0.111_2	0.50329_3	0.123_3	8.1_2	0.016	0.12	0.26
NAT	0.257_2	0.5554_5	0.276_3	3.62_4	0.79	2.3	3.0
NAT-1	0	0	n.d.	n.d.	0	0	n.d.
NAT-2	0	0	n.d.	n.d.	0	0	n.d.
NAT-4	0	0	n.d.	n.d.	0	0	n.d.
NES	0.368_2	0.5203_3	0.538_5	1.86_2	0.82	1.4	0.87
NON*	0.326_3	0.5172_3	0.45_1	2.22_3	0.49	1.0	0.80
NPO	0.134_2	0.50144_3	0.154_3	6.5_1	0.0088	0.057	0.11
NPT	0.430_3	0.520_1	0.70_1	1.44_2	1.6	2.1	0.75
NSI*	0.0038_1	0.5	0.0038_1	260_5	0.000039	0.0070	0.039
OBW	0.447_2	0.519_1	0.75_1	1.33_2	2.0	2.5	0.71
OFF	0.43_1	0.513_1	0.71_2	1.41_4	1.0	1.4	0.48
OKO	0.433_2	0.5107_3	0.73_1	1.36_1	1.0	1.3	0.41
OSI	0.338_3	0.5123_2	0.49_1	2.06_2	0.40	0.78	0.56
OSO	0.362_1	0.5351_3	0.494_3	2.03_1	1.2	2.2	1.5
OWE	0.501_2	0.4998_3	1.01_1	0.99_1	1.0	1.0	0.0056
PAU	0.590_2	0.475_1	1.59_2	0.63_1	2.1	1.5	0.97
PCR	0.530_3	0.4965_3	1.15_1	0.87_1	0.89	0.79	0.12
PHI	0.535_3	0.493_1	1.18_2	0.85_1	1.5	1.3	0.25
PON	0.416_2	0.5117_3	0.68_1	1.47_2	0.84	1.2	0.46

POS	0.418_3	0.519_1	0.66_1	1.50_2	1.3	1.8	0.75
PSI	0.448_1	0.5028_1	0.803_4	1.25_1	0.38	0.46	0.10
PUN	0.425_3	0.521_1	0.68_1	1.47_2	1.5	2.1	0.80
RHO	0.602_3	0.458_1	1.79_3	0.56_1	2.9	1.9	1.7
RRO	0.224_2	0.5251_2	0.261_3	3.83_4	0.31	1.1	1.4
RRO-1	0.221	0.779	0.08	12	0.44	1.5	3.9
RSN	0.646_4	0.4819_5	1.96_3	0.51_1	1.2	0.66	0.80
RTE	0.315_4	0.5226_5	0.42_1	2.38_5	0.57	1.2	1.1
RTH	0.379_3	0.524_1	0.55_1	1.80_3	1.1	1.7	1.0
RUT-1*	0.412_3	0.5110_3	0.67_1	1.49_2	0.76	1.1	0.44
RWR*	0.942_1	0.49900_1	16.4_4	0.061_2	0.035	0.0022	0.099
RWY	0.469_1	0.539_2	0.75_1	1.33_2	4.3	4.9	1.4
SAF	0.470_1	0.5027_1	0.876_5	1.14_1	0.66	0.74	0.098
SAO	0.404_2	0.5281_5	0.607_5	1.65_1	1.5	2.2	1.1
SAS	0.397_3	0.522_1	0.60_1	1.66_3	1.2	1.8	0.90
SAT*	0.427_2	0.5109_4	0.71_1	1.40_2	0.92	1.2	0.42
SAV	0.419_2	0.5190_4	0.67_1	1.50_1	1.3	1.8	0.74
SBE	0.462_2	0.5122_5	0.82_1	1.23_1	1.8	2.2	0.44
SBN	0.719_3	0.4610_5	3.00_4	0.333_5	1.8	0.70	2.0
SBS	0.433_1	0.5221_4	0.699_5	1.43_1	1.8	2.3	0.84
SBT	0.432_2	0.522_1	0.70_1	1.44_2	1.8	2.3	0.84
SEW	0.52_1	0.497_1	1.08_3	0.93_3	1.4	1.3	0.10
SFE	0.414_3	0.5125_4	0.67_1	1.49_2	0.88	1.2	0.49
SFF	0.357_2	0.5205_2	0.512_4	1.95_2	0.74	1.3	0.90
SFG	0.455_5	0.506_1	0.82_2	1.22_3	0.84	1.0	0.20
SFH	0.391_3	0.5154_4	0.60_1	1.66_2	0.81	1.3	0.63
SFN	0.384_3	0.5163_4	0.58_1	1.71_2	0.79	1.3	0.68

SFO	0.442_4	0.515_1	0.75_1	1.34_3	1.5	1.9	0.57
SFS	0.454_4	0.509_1	0.80_2	1.25_2	1.2	1.4	0.32
SFV	0.478	0.522	0.838	1.2	1.1	1.2	0.21
SFV-1	0.489	0.511	0.914	1.1	1.1	1.2	0.11
SFW	0.454_1	0.5107_3	0.80_1	1.26_1	1.4	1.7	0.39
SGT*	0.356_3	0.5195_4	0.51_1	1.95_3	0.71	1.3	0.86
SIV	0.522_4	0.494_1	1.12_2	0.89_2	1.8	1.6	0.20
SOD*	0.473_4	0.505_1	0.88_2	1.14_2	1.3	1.5	0.19
SOF	0.536_1	0.4908_3	1.20_1	0.835_5	1.8	1.6	0.33
SOS	0.368_2	0.5113_2	0.556_5	1.80_2	0.48	0.83	0.49
SSF	0.439_2	0.5102_4	0.75_1	1.33_2	1.0	1.3	0.38
SSY	0.399_2	0.5134_2	0.628_5	1.59_1	0.78	1.2	0.55
STF	0.378_2	0.5225_4	0.56_1	1.80_2	0.98	1.6	0.95
STI	0.416_2	0.5135_3	0.67_1	1.48_1	0.96	1.3	0.53
STO	0.434_2	0.5063_2	0.75_1	1.34_1	0.63	0.82	0.24
STT	0.425_2	0.5126_3	0.704_5	1.42_1	1.0	1.4	0.49
STW	0.413_1	0.5215_3	0.645_4	1.55_1	1.4	1.9	0.85
SVV*	0.382_4	0.5141_5	0.58_1	1.71_4	0.68	1.1	0.59
SZR	0.417_2	0.5072_2	0.70_1	1.44_1	0.56	0.78	0.28
TER	0.456_4	0.508_1	0.81_2	1.23_2	1.2	1.4	0.29
THO	0.447_4	0.513_1	0.77_1	1.30_2	1.5	1.8	0.48
TOL*	0.634_4	0.483_1	1.85_4	0.54_1	1.2	0.67	0.71
TON	0.387_2	0.5111_2	0.604_5	1.65_1	0.58	0.92	0.46
TSC	0.467_3	0.511_1	0.84_1	1.19_2	2.0	2.3	0.40
TUN	0.433_2	0.5107_4	0.73_1	1.36_1	1.0	1.3	0.41
UEI	0.811_1	0.4426_2	5.41_4	0.185_1	2.1	0.49	3.5
UFI	0.46_1	0.512_2	0.80_3	1.25_5	1.6	1.9	0.44

UOS	0.511_3	0.4985_4	1.05_1	0.95_1	0.99	0.94	0.049
UOV	0.429_2	0.5136_3	0.71_1	1.41_1	1.1	1.5	0.52
UOZ*	0.552_3	0.4942_3	1.26_2	0.79_1	0.91	0.74	0.21
USI	0.368_2	0.5314_5	0.51_1	1.95_2	1.2	2.0	1.3
UTL	0.440_3	0.514_1	0.74_1	1.35_2	1.4	1.8	0.54
UWY	0.453_3	0.510_1	0.80_1	1.25_2	1.3	1.6	0.35
VET	0.370_2	0.5083_1	0.568_5	1.76_2	0.37	0.63	0.36
VFI	0.419_2	0.5185_4	0.67_1	1.49_1	1.3	1.8	0.72
VNI*	0.477_3	0.5010_2	0.91_1	1.10_2	0.35	0.38	0.036
VSV	0.452_4	0.5025_2	0.82_2	1.22_2	0.38	0.46	0.092
WEI	0.224_2	0.50211_4	0.286_3	3.50_3	0.028	0.098	0.12
YUG*	0.480_3	0.5025_3	0.92_1	1.09_1	0.90	0.98	0.086
ZON	0.478_2	0.5031_3	0.91_1	1.10_1	0.99	1.1	0.11

Table S5: Compositions, selectivities, loadings [in mmol g^{-1}], and performance criteria [in mmol g^{-1}] for all zeolites from the IZA database used in the screening study using the TraPPE–UA force field at $T = 300$ K, $p = 20$ bar, and $z_F = 0.5$. Subscript(s) indicate uncertainty in the last digit(s). "n.d." indicates "not defined". Asterisk after the framework type in the first column indicates that the largest pore window for this framework, obtained from the IZA–SC database,[4] is 3.4 Å. The idealized all-silica zeolite topologies are represented as XXX, while XXX-i ($i = 1, 2, ...$) corresponds to an experimental structure.

zeolite	$x_{C_2H_4}$	$y_{C_2H_4}$	$S_{C_2H_4}$	$S_{C_2H_6}$	$Q_{C_2H_4}$	$Q_{C_2H_6}$	P
ABW	0.893_1	0.4999426_4	8.3_1	0.120_1	0.0021	0.00017	0.0044
ACO	0.732_2	0.4734_4	3.04_4	0.329_4	1.3	0.46	1.4
AEI	0.431_2	0.5165_5	0.71_1	1.41_1	1.4	1.8	0.63
AEL	0.398_3	0.5101_3	0.63_1	1.58_2	0.60	0.91	0.41
AEN	0.801_3	0.499686_5	4.0_1	0.248_4	0.014	0.0034	0.019
AET	0.410_4	0.5094_4	0.67_1	1.49_3	0.65	0.93	0.37
AFG*	0.358_4	0.5195_5	0.52_1	1.94_4	0.72	1.3	0.85
AFI	0.416_2	0.5101_3	0.68_1	1.46_2	0.74	1.0	0.40
AFN*	0.430_2	0.5073_2	0.73_1	1.37_1	0.68	0.90	0.28
AFO	0.379_3	0.5123_3	0.58_1	1.72_2	0.58	0.96	0.52
AFR	0.417_3	0.520_1	0.66_1	1.52_2	1.3	1.9	0.78
AFS	0.444_1	0.5169_4	0.75_1	1.34_1	1.7	2.1	0.63
AFT	0.390_4	0.523_1	0.58_1	1.71_3	1.1	1.7	0.93
AFX-1	0.403_2	0.5191_4	0.63_1	1.60_2	1.1	1.6	0.77
AFY	0.475_3	0.513_1	0.86_1	1.16_2	2.7	3.0	0.45
AHT*	0.032_1	0.4999992	0.033_1	31_1	0.000022	0	n.d.
ANA*	0.000056_2	0.5	n.d.	n.d.	0	0	n.d.
APC*	0.755_4	0.49764_5	3.1_1	0.32_1	0.12	0.037	0.13
APD	0.819_2	0.4434_5	5.7_1	0.176_3	2.1	0.45	3.6
AST*	0.387_1	0.5175_2	0.589_4	1.70_1	0.87	1.4	0.73

ASV	0.374_2	0.5139_3	0.57_1	1.77_2	0.62	1.0	0.59
ATN	0.356_1	0.5205_1	0.509_1	1.96_1	0.74	1.3	0.90
ATO	0.373_2	0.5114_1	0.567_4	1.76_1	0.51	0.86	0.49
ATS	0.383_3	0.5222_5	0.57_1	1.76_2	1.0	1.6	0.93
ATT	0.409_2	0.5181_5	0.64_1	1.56_2	1.1	1.6	0.72
ATV	0.766_3	0.4664_4	3.7_1	0.27_1	1.4	0.44	1.9
AWO	0.622_3	0.4771_5	1.80_3	0.55_1	1.6	1.0	0.97
AWW	0.32_1	0.517_1	0.44_2	2.3_1	0.47	0.99	0.81
BCT*	0	0.5	0	n.d.	0	0	n.d.
BEA	0.395_3	0.526_1	0.59_1	1.70_2	1.3	2.0	1.0
BEC	0.374_3	0.530_1	0.53_1	1.89_2	1.2	2.0	1.3
BIK	0.968_1	0.4999543_2	30_1	0.033_1	0.0016	0.00012	0.0056
BOF	0.410_2	0.5177_4	0.65_1	1.54_2	1.1	1.6	0.70
BOG	0.403_3	0.521_1	0.62_1	1.61_2	1.2	1.7	0.83
BOZ	0.463_2	0.512_1	0.82_1	1.22_1	1.9	2.2	0.43
BPH	0.398_2	0.525_1	0.60_1	1.68_2	1.3	2.0	1.0
BRE*	0.368_4	0.5187_5	0.54_1	1.85_3	0.76	1.3	0.80
BSV	0.525_4	0.495_1	1.13_2	0.89_2	1.4	1.3	0.16
CAN	0.355_2	0.5142_2	0.52_1	1.93_2	0.53	0.96	0.63
CAS*	0.810_1	0.4513_2	5.18_4	0.193_2	1.8	0.43	3.0
CDO	0.350_2	0.5186_3	0.50_1	2.00_2	0.64	1.2	0.83
CFI	0.414_5	0.510_1	0.68_2	1.47_4	0.71	1.0	0.39
CGF*	0.364_4	0.5169_4	0.53_1	1.87_3	0.67	1.2	0.73
CGS	0.330_2	0.5241_3	0.447_4	2.24_2	0.68	1.4	1.1
CON	0.39_1	0.525_1	0.57_2	1.75_5	1.2	1.8	1.0
CSV	0.409_2	0.5196_5	0.64_1	1.57_2	1.2	1.7	0.78
CZP	0.907_2	0.49830_2	9.8_2	0.102_2	0.063	0.0064	0.14

DAC	0.518_3	0.496_1	1.09_2	0.91_1	1.5	1.4	0.13
DDR	0.590_2	0.4828_4	1.54_2	0.65_1	1.6	1.1	0.68
DFO	0.403_3	0.526_1	0.61_1	1.65_2	1.4	2.1	1.1
DFT	0.689_2	0.4450_5	2.76_2	0.362_3	2.6	1.2	2.6
DOH*	0.437_5	0.516_1	0.73_2	1.37_3	1.5	1.9	0.61
DON	0.415_4	0.512_1	0.68_1	1.48_3	0.83	1.2	0.45
EAB	0.336_4	0.532_1	0.44_1	2.25_5	0.92	1.8	1.5
EDI	0.398_1	0.5253_4	0.598_4	1.67_1	1.3	2.0	1.0
EEI*	0.333_4	0.5143_3	0.47_1	2.12_4	0.44	0.88	0.66
EMT	0.43_1	0.531_3	0.66_3	1.5_1	2.1	2.8	1.2
EON	0.445_2	0.5080_3	0.78_1	1.29_1	0.94	1.2	0.30
EPI	0.400_4	0.520_1	0.62_1	1.62_3	1.1	1.7	0.80
ERI	0.368_5	0.524_1	0.53_1	1.89_5	0.95	1.6	1.0
ESV	0.313_2	0.5173_2	0.426_4	2.35_2	0.44	0.97	0.83
ETR	0.380_3	0.524_1	0.56_1	1.79_3	1.0	1.7	0.99
EUO	0.364_4	0.5179_5	0.53_1	1.88_3	0.70	1.2	0.78
EZT	0.388_2	0.5212_4	0.582_5	1.72_2	1.0	1.6	0.88
FAR*	0.334_4	0.527_1	0.45_1	2.22_5	0.77	1.5	1.2
FAU	0.420_2	0.534_1	0.63_1	1.58_1	2.1	2.9	1.3
FER	0.38_1	0.518_1	0.58_2	1.7_1	0.87	1.4	0.77
FRA*	0.348_4	0.531_1	0.47_1	2.13_5	0.98	1.8	1.4
GIS*	0.508_4	0.497_1	1.04_2	0.96_2	2.0	2.0	0.089
GIU*	0.334_4	0.523_1	0.46_1	2.18_5	0.67	1.3	1.0
GME	0.426_2	0.5166_4	0.70_1	1.44_1	1.3	1.8	0.64
GON	0.382_2	0.5087_2	0.60_1	1.67_2	0.44	0.71	0.37
GOO*	0.483_3	0.5019_3	0.93_1	1.08_1	0.81	0.87	0.067
HEU	0.426_1	0.5144_3	0.701_5	1.43_1	1.2	1.6	0.55

IFO	0.396_3	0.5140_4	0.62_1	1.61_2	0.78	1.2	0.57
IFR	0.338_2	0.5232_3	0.465_5	2.15_3	0.70	1.4	1.1
IFW	0.424_4	0.518_1	0.69_1	1.46_3	1.3	1.8	0.68
IFY	0.398_4	0.5151_5	0.62_1	1.61_3	0.86	1.3	0.62
IHW	0.368_3	0.5137_3	0.55_1	1.82_3	0.58	0.99	0.59
IMF	0.407_3	0.5163_5	0.64_1	1.56_2	1.0	1.5	0.65
IRN	0.408_5	0.522_1	0.63_2	1.58_4	1.3	1.9	0.86
IRR	0.429_2	0.533_1	0.66_1	1.52_2	2.3	3.0	1.3
ISV	0.380_2	0.5287_5	0.55_1	1.83_2	1.2	2.0	1.2
ITE	0.447_2	0.5127_5	0.77_1	1.30_1	1.4	1.8	0.47
ITG	0.381_3	0.5186_5	0.57_1	1.75_3	0.86	1.4	0.78
ITH	0.36_1	0.518_1	0.53_2	1.9_1	0.70	1.2	0.78
ITR	0.358_2	0.5178_2	0.520_5	1.92_2	0.66	1.2	0.78
ITT	0.426_2	0.532_1	0.65_1	1.53_2	2.2	2.9	1.2
ITW	0.487_4	0.5012_4	0.94_2	1.06_2	0.70	0.73	0.042
IWR	0.384_3	0.526_1	0.56_1	1.78_3	1.2	1.9	1.1
IWS	0.396_2	0.5248_4	0.59_1	1.69_2	1.3	1.9	1.0
IWV	0.428_1	0.5199_2	0.692_3	1.44_1	1.6	2.1	0.76
IWW	0.391_4	0.519_1	0.60_1	1.68_3	0.96	1.5	0.77
JBW	0.857_1	0.499788_1	5.99_5	0.167_1	0.0084	0.0013	0.015
JNT*	0.640_3	0.4911_2	1.85_2	0.54_1	0.63	0.35	0.39
JOZ	0.455_3	0.510_1	0.80_1	1.24_2	1.4	1.6	0.36
JRY	0.455_3	0.508_1	0.81_1	1.24_2	1.1	1.3	0.28
JSN	0.379_3	0.5173_4	0.57_1	1.75_3	0.79	1.3	0.73
JSR	0.443_2	0.531_1	0.70_1	1.42_2	2.6	3.3	1.1
JST	0.447_4	0.515_1	0.76_2	1.31_3	1.6	2.0	0.54
JSW*	0.342_3	0.5143_3	0.49_1	2.03_3	0.47	0.91	0.64

KFI	0.391_3	0.522_1	0.59_1	1.71_3	1.1	1.7	0.92
LAU	0.412_2	0.5153_3	0.66_1	1.52_1	1.0	1.4	0.60
LEV	0.327_4	0.5227_5	0.44_1	2.26_4	0.63	1.3	1.1
LIO*	0.450_4	0.507_1	0.79_2	1.26_3	0.97	1.2	0.27
LOS*	0.399_2	0.5184_3	0.62_1	1.62_2	1.0	1.5	0.75
LOV	0.683_2	0.4741_2	2.39_2	0.419_3	1.4	0.66	1.2
LTA	0.404_4	0.533_1	0.59_1	1.68_3	1.7	2.6	1.3
LTF	0.33_1	0.519_1	0.46_1	2.2_1	0.58	1.2	0.89
LTJ*	0.9568_4	0.499778_2	22.2_2	0.0451_4	0.0078	0.00037	0.024
LTL	0.393_3	0.5166_5	0.61_1	1.65_3	0.88	1.4	0.68
LTN*	0.337_5	0.526_1	0.46_1	2.2_1	0.78	1.5	1.2
MAR*	0.346_3	0.5225_4	0.48_1	2.07_3	0.73	1.4	1.0
MAZ	0.34_1	0.520_1	0.48_2	2.1_1	0.64	1.2	0.90
MEI	0.378_2	0.536_1	0.53_1	1.90_2	1.4	2.4	1.5
MEL	0.397_4	0.517_1	0.61_1	1.63_3	0.96	1.5	0.71
MEP*	0.418_3	0.517_1	0.67_1	1.49_2	1.2	1.7	0.67
MER	0.509_3	0.4987_4	1.04_2	0.96_1	0.96	0.92	0.040
MFI	0.427_2	0.5115_4	0.71_1	1.41_2	0.97	1.3	0.44
MFS	0.401_3	0.5122_4	0.64_1	1.57_2	0.73	1.1	0.49
MON	0.45_1	0.4999429_5	0.83_5	1.2_1	0.0022	0.00026	0.000048
MOR	0.530_4	0.494_1	1.15_2	0.87_2	1.4	1.2	0.19
MOZ	0.380_3	0.5176_4	0.57_1	1.75_2	0.81	1.3	0.74
MRE	0.354_2	0.5125_2	0.521_5	1.92_2	0.46	0.85	0.55
MSE	0.383_3	0.5203_4	0.57_1	1.74_2	0.95	1.5	0.85
MSO*	0.398_3	0.5123_4	0.63_1	1.59_2	0.71	1.1	0.50
MTN*	0.428_2	0.5154_4	0.70_1	1.42_1	1.3	1.7	0.59
MTT	0.334_3	0.5150_2	0.47_1	2.12_3	0.46	0.92	0.69

MTW	0.370_3	0.5107_3	0.56_1	1.77_3	0.47	0.80	0.46
MVY*	0	0.5	0	n.d.	0	0	n.d.
MWW	0.416_2	0.5189_4	0.66_1	1.51_1	1.3	1.8	0.74
NAB	0.44_1	0.4999586_3	0.79_3	1.27_5	0.0017	0.00038	0.000090
NAT	0.476_1	0.5050_3	0.89_1	1.12_1	1.4	1.5	0.17
NES	0.380_3	0.5187_4	0.57_1	1.76_2	0.85	1.4	0.78
NON*	0.342_1	0.5155_1	0.489_3	2.04_1	0.51	0.98	0.70
NPO	0.60_1	0.499953_1	1.47_5	0.68_2	0.0022	0.00061	0.00084
NPT	0.39_1	0.529_2	0.58_2	1.73_5	1.4	2.2	1.2
NSI*	0.074_2	0.4999966	0.080_3	12.5_4	0.00012	0	n.d.
OBW	0.421_2	0.530_1	0.65_1	1.55_2	1.9	2.7	1.2
OFF	0.333_3	0.528_1	0.45_1	2.25_4	0.80	1.6	1.3
OKO	0.398_5	0.518_1	0.62_1	1.63_4	0.99	1.5	0.73
OSI	0.368_3	0.5098_3	0.56_1	1.79_3	0.42	0.73	0.42
OSO	0.431_3	0.516_1	0.71_1	1.41_2	1.4	1.8	0.63
OWE	0.337_5	0.523_1	0.46_1	2.16_5	0.70	1.4	1.1
PAU	0.46_1	0.506_1	0.84_2	1.20_3	1.1	1.3	0.23
PCR	0.496_2	0.5005_3	0.98_1	1.02_1	0.95	0.96	0.018
PHI	0.400_4	0.515_1	0.63_1	1.59_3	0.85	1.3	0.59
PON	0.506_5	0.499_1	1.03_2	0.97_2	1.3	1.2	0.036
POS	0.382_2	0.5274_4	0.555_5	1.80_2	1.2	1.9	1.1
PSI	0.375_3	0.5069_2	0.58_1	1.71_2	0.33	0.55	0.29
PUN	0.37_1	0.537_2	0.50_2	2.0_1	1.3	2.3	1.6
RHO	0.507_3	0.497_1	1.04_2	0.96_2	2.2	2.1	0.082
RRO	0.548_4	0.4981_2	1.22_2	0.82_2	0.35	0.29	0.071
RSN	0.656_2	0.4848_2	2.02_2	0.494_5	0.97	0.51	0.69
RTE	0.350_3	0.5158_3	0.50_1	1.98_3	0.55	1.0	0.70

RTH	0.432_{2}	0.5120_{5}	0.73_{1}	1.38_{2}	1.1	1.4	0.46
RUT-1*	0.295_{1}	0.5256_{2}	0.377_{3}	2.65_{2}	0.54	1.3	1.3
RWR*	0.813_{3}	0.4922_{1}	4.5_{1}	0.222_{4}	0.33	0.075	0.49
RWY	0.452_{1}	0.559_{1}	0.650_{5}	1.54_{1}	4.1	5.0	2.2
SAF	0.413_{3}	0.5085_{3}	0.68_{1}	1.47_{2}	0.61	0.87	0.34
SAO	0.404_{2}	0.527_{1}	0.61_{1}	1.65_{2}	1.5	2.2	1.1
SAS	0.417_{3}	0.5168_{5}	0.67_{1}	1.50_{2}	1.2	1.6	0.66
SAT*	0.335_{2}	0.5238_{3}	0.458_{5}	2.19_{2}	0.70	1.4	1.1
SAV	0.419_{3}	0.517_{1}	0.67_{1}	1.48_{2}	1.2	1.7	0.68
SBE	0.434_{3}	0.521_{1}	0.71_{1}	1.42_{2}	1.7	2.3	0.79
SBN	0.758_{1}	0.4205_{5}	4.31_{4}	0.232_{2}	3.0	0.95	4.3
SBS	0.416_{2}	0.528_{1}	0.64_{1}	1.57_{2}	1.8	2.5	1.1
SBT	0.420_{1}	0.5258_{2}	0.653_{2}	1.531_{5}	1.7	2.4	1.0
SEW	0.404_{3}	0.5191_{5}	0.63_{1}	1.59_{2}	1.1	1.6	0.77
SFE	0.401_{3}	0.5154_{4}	0.63_{1}	1.59_{2}	0.89	1.3	0.62
SFF	0.413_{3}	0.5121_{4}	0.67_{1}	1.49_{2}	0.84	1.2	0.48
SFG	0.400_{1}	0.5129_{2}	0.632_{4}	1.58_{1}	0.76	1.1	0.52
SFH	0.392_{2}	0.5150_{3}	0.61_{1}	1.65_{2}	0.80	1.2	0.61
SFN	0.393_{4}	0.515_{1}	0.61_{1}	1.64_{3}	0.79	1.2	0.60
SFO	0.433_{3}	0.515_{1}	0.72_{1}	1.39_{2}	1.3	1.7	0.57
SFS	0.415_{4}	0.517_{1}	0.66_{1}	1.51_{3}	1.2	1.6	0.67
SFW	0.414_{3}	0.518_{1}	0.66_{1}	1.53_{2}	1.2	1.7	0.73
SGT*	0.403_{1}	0.5127_{2}	0.642_{4}	1.56_{1}	0.78	1.2	0.51
SIV	0.468_{3}	0.507_{1}	0.85_{1}	1.17_{2}	1.4	1.6	0.26
SOD*	0.300_{3}	0.540_{1}	0.37_{1}	2.73_{5}	0.83	1.9	1.9
SOF	0.451_{3}	0.512_{1}	0.78_{1}	1.28_{2}	1.5	1.8	0.46
SOS	0.483_{3}	0.5013_{3}	0.93_{1}	1.08_{2}	0.59	0.63	0.046

SSF	0.394_{2}	0.5179_{4}	0.61_{1}	1.65_{2}	0.95	1.5	0.73
SSY	0.410_{4}	0.513_{1}	0.66_{1}	1.52_{3}	0.86	1.2	0.52
STF	0.433_{3}	0.513_{1}	0.73_{1}	1.38_{2}	1.2	1.5	0.49
STI	0.383_{3}	0.520_{1}	0.57_{1}	1.75_{3}	0.94	1.5	0.85
STO	0.420_{3}	0.5081_{3}	0.70_{1}	1.43_{2}	0.64	0.89	0.32
STT	0.406_{2}	0.5154_{4}	0.64_{1}	1.55_{2}	0.96	1.4	0.62
STW	0.429_{3}	0.519_{1}	0.70_{1}	1.43_{2}	1.5	2.0	0.71
SVV*	0.297_{3}	0.5244_{3}	0.38_{1}	2.61_{4}	0.53	1.3	1.2
SZR	0.472_{1}	0.5030_{1}	0.884_{5}	1.13_{1}	0.78	0.87	0.11
TER	0.418_{3}	0.516_{1}	0.67_{1}	1.49_{2}	1.2	1.6	0.64
THO	0.396_{1}	0.5254_{3}	0.592_{4}	1.69_{1}	1.3	2.0	1.0
TOL*	0.436_{3}	0.5095_{5}	0.74_{1}	1.35_{2}	0.94	1.2	0.36
TON	0.406_{4}	0.5100_{4}	0.66_{1}	1.52_{3}	0.66	0.96	0.40
TSC	0.437_{5}	0.522_{2}	0.71_{2}	1.41_{4}	1.9	2.4	0.82
TUN	0.400_{3}	0.517_{1}	0.62_{1}	1.60_{3}	0.98	1.5	0.69
UEI	0.56_{1}	0.489_{1}	1.35_{4}	0.74_{2}	1.4	1.1	0.43
UFI	0.39_{1}	0.530_{2}	0.56_{3}	1.8_{1}	1.4	2.2	1.3
UOS	0.482_{4}	0.503_{1}	0.92_{2}	1.09_{2}	1.1	1.2	0.099
UOV	0.379_{2}	0.5235_{4}	0.56_{1}	1.80_{2}	1.0	1.7	0.99
UOZ*	0.358_{3}	0.5157_{3}	0.52_{1}	1.91_{3}	0.59	1.1	0.69
USI	0.415_{2}	0.5206_{5}	0.65_{1}	1.53_{2}	1.3	1.9	0.81
UTL	0.405_{3}	0.523_{1}	0.62_{1}	1.62_{3}	1.3	2.0	0.94
UWY	0.411_{4}	0.520_{1}	0.64_{1}	1.55_{3}	1.2	1.8	0.77
VET	0.342_{4}	0.5099_{3}	0.50_{1}	2.00_{4}	0.34	0.65	0.45
VFI	0.430_{2}	0.516_{1}	0.71_{1}	1.41_{2}	1.4	1.8	0.61
VNI*	0.673_{3}	0.4919_{1}	2.12_{3}	0.47_{1}	0.50	0.24	0.38
VSV	0.584_{3}	0.4973_{1}	1.42_{2}	0.70_{1}	0.30	0.21	0.11

WEI	0.748_3	0.49910_1	2.98_5	0.335_5	0.045	0.015	0.049
YUG*	0.494_2	0.5006_2	0.98_1	1.03_1	0.75	0.77	0.019
ZON	0.330_4	0.5242_5	0.45_1	2.24_4	0.68	1.4	1.1

Table S6: Pure-component loading [in molecules/uc] in MFI-1 at $T = 303$ K.

	Ethylene		Ethane		
p	UA	UA2	UA	UA2	EH
0.001	0.031_1	0.037_1	0.063_2	0.058_1	0.062_1
0.01	0.31_1	0.37_1	0.60_2	0.56_1	0.61_1
0.1	2.81_4	3.2_1	4.9_1	4.33_5	5.02_5
0.2	4.9_1	5.2_1	7.34_6	6.4_1	7.40_3
0.5	8.2_1	8.1_1	9.76_4	8.75_3	9.74_3
1	10.17_3	9.85_4	10.89_4	9.94_3	10.79_2
1.5	11.1_1	10.56_4	11.40_2	10.45_3	11.21_3
2	11.65_5	10.98_4	11.70_3	10.74_2	11.44_1
5	13.25_5	12.05_4	12.58_5	11.44_2	12.00_2
10	14.3_1	12.77_4	13.4_1	11.79_1	12.44_4
20	15.01_4	13.52_5	14.1_1	12.07_3	13.00_4
30	15.34_3	14.0_1	14.5_1	12.20_2	13.4_1
40	15.52_3	14.27_5	14.66_4	12.33_3	13.5_1
50	15.64_3	14.4_1	14.78_5	12.38_4	13.8_1
100	15.88_4	14.8_1	14.93_3	12.41_3	13.9_1

Subscript(s) indicate uncertainty in the last digit(s).

Table S7: Pure-component loading [in molecules/uc] in MFI-0 and MFI-2 using TraPPE–UA2 force field at $T = 303$ K.

	Ethylene		Ethane	
p	MFI-0	MFI-2	MFI-0	MFI-2
0.001	0.0178_4	0.0277_5	0.0381_4	0.048_1
0.01	0.175_5	0.271_4	0.372_5	0.467_5
0.1	1.66_4	2.48_2	3.03_3	3.77_4
0.2	3.03_5	4.32_5	4.87_3	5.83_4
0.5	5.71_6	7.37_3	7.38_3	8.30_4
1	7.91_8	9.33_3	8.86_2	9.62_2
1.5	8.95_5	10.23_4	9.52_2	10.21_2
2	9.52_5	10.76_3	9.93_2	10.55_2
5	11.06_4	12.15_2	10.91_1	11.36_1
10	11.89_3	13.01_3	11.43_1	11.80_1
20	12.58_4	13.81_4	11.81_1	12.17_2
30	12.93_7	14.21_4	12.00_1	12.38_2
40	13.15_5	14.45_4	12.11_2	12.49_2
50	13.30_5	14.63_3	12.12_1	12.55_2
100	13.58_3	14.90_4		

Subscript(s) indicate uncertainty in the last digit(s).

Table S8: Pure-component loading [in molecules/uc] in CHA at $T = 303$ K.

	Ethylene		Ethane	
p	UA	UA2	UA	UA2
0.001	0.0087_2	0.0104_3	0.0193_5	0.0173_4
0.01	0.087_1	0.101_2	0.188_5	0.169_1
0.1	0.78_2	0.92_1	1.48_3	1.41_3
0.2	1.40_2	1.61_3	2.39_3	2.34_5
0.5	2.64_4	3.01_2	3.75_2	3.76_4
1	3.70_2	4.10_4	4.62_4	4.67_2
1.5	4.27_1	4.61_3	5.01_1	5.03_2
2	4.61_2	4.92_1	5.24_1	5.28_1
5	5.37_1	5.53_1	5.66_1	5.70_1
10	5.67_1	5.781_2	5.82_1	5.87_1
20	5.85_1	5.930_4	5.911_1	5.96_1
30	5.920_4	6.00_1	5.939_2	6.010_4
40	5.959_4	6.04_1	5.954_2	6.042_4
50	5.99_1	6.078_5	5.961_1	6.05_1
100	6.042_4	6.14_1		

Subscript(s) indicate uncertainty in the last digit(s).

Table S9: Pure-component loading [in molecules/uc] in DDR at $T = 303$ K.

	Ethylene		Ethane	
p	UA	UA2	UA	UA2
0.001	0.0355_6	0.040_1	0.087_1	0.080_2
0.01	0.34_1	0.39_1	0.77_1	0.73_1
0.1	2.45_3	2.72_6	3.96_4	3.87_3
0.2	3.72_5	4.06_4	5.16_3	5.09_3
0.5	5.59_5	6.01_4	6.64_4	6.65_4
1	7.00_3	7.45_7	7.82_4	7.90_5
1.5	7.81_3	8.35_2	8.53_4	8.61_3
2	8.36_6	8.87_5	9.03_5	9.18_4
5	9.99_3	10.36_6	10.45_2	10.51_4
10	10.84_3	11.08_4	11.10_2	11.17_2
20	11.35_3	11.53_2	11.50_1	11.56_1
30	11.56_2	11.69_1	11.63_2	11.70_1
40	11.67_2	11.79_1	11.70_1	11.79_1
50	11.73_1	11.85_1	11.74_2	11.81_1
100	11.86_1	11.95_1		

Subscript(s) indicate uncertainty in the last digit(s).

Table S10: Pure-component loading [in molecules/uc] in AEI at $T = 303$ K.

	Ethylene		Ethane	
p	UA	UA2	UA	UA2
0.001	0.0073_2	0.0087_1	0.0149_4	0.0145_4
0.01	0.073_2	0.085_1	0.145_3	0.144_2
0.1	0.65_1	0.77_1	1.20_2	1.20_2
0.2	1.20_2	1.39_1	1.96_2	2.03_2
0.5	2.35_3	2.74_2	3.26_2	3.44_3
1	3.48_3	4.14_3	4.30_4	4.71_3
1.5	4.21_4	5.08_3	4.92_5	5.50_5
2	4.77_4	5.81_2	5.41_5	6.01_5
5	6.69_4	8.21_4	7.06_3	7.78_5
10	8.17_7	9.70_2	8.37_4	8.97_8
20	9.50_6	10.75_2	9.43_6	10.01_5
30	10.11_4	11.18_2	9.98_7	10.44_5
40	10.48_4	11.40_1	10.32_3	10.76_4
50	10.74_3	11.54_2	10.46_4	10.82_6
100	11.23_3	11.79_2		

Subscript(s) indicate uncertainty in the last digit(s).

Table S11: Pure-component loading [in molecules/uc] in STT at $T = 303$ K.

	Ethylene		Ethane	
p	UA	UA2	UA	UA2
0.001	0.0165_4	0.0190_4	0.038_1	0.0363_6
0.01	0.164_3	0.183_2	0.354_5	0.35_1
0.1	1.38_1	1.54_2	2.45_3	2.46_3
0.2	2.36_2	2.58_2	3.72_4	3.74_3
0.5	4.12_6	4.40_5	5.40_4	5.49_2
1	5.45_3	5.75_2	6.41_3	6.55_3
1.5	6.14_2	6.42_1	6.88_2	7.01_2
2	6.59_5	6.81_1	7.17_2	7.27_2
5	7.65_2	7.81_1	7.76_1	7.91_2
10	8.25_2	8.41_1	8.06_1	8.31_2
20	8.89_3	9.05_2	8.37_2	8.74_3
30	9.26_3	9.44_2	8.57_3	9.03_3
40	9.51_5	9.69_2	8.71_3	9.24_7
50	9.74_4	9.88_2	8.81_3	9.29_3
100	10.12_5	10.24_3		

Subscript(s) indicate uncertainty in the last digit(s).

Table S12: Pure-component loading [in molecules/uc] in DFT at $T = 303$ K.

	Ethylene		Ethane		
p	UA	UA2	UA	UA2	EH
0.001	0.00023_1	0.00053_2			
0.01	0.00236_4	0.0052_1	0.00076_1		
0.1	0.0237_3	0.052_1	0.0074_1	0.00107_2	0.00072_1
0.2	0.0477_5	0.104_1	0.0148_3	0.00211_4	0.00145_3
0.5	0.123_2	0.27_1	0.037_1	0.0052_1	0.0036_1
1	0.260_4	0.53_1	0.077_2	0.0106_3	0.0071_2
1.5	0.415_4	0.79_1	0.118_1	0.0153_4	0.0106_3
2	0.58_1	1.01_1	0.161_3	0.0208_3	0.0142_5
5	1.33_1	1.59_1	0.46_1	0.051_1	0.035_1
10	1.688_4	1.801_5	1.07_1	0.099_2	0.070_1
20	1.850_1	1.898_2	1.60_1	0.185_2	0.137_3
30	1.897_2	1.930_1	1.743_5	0.258_4	0.197_5
40	1.919_1	1.944_2	1.801_3	0.32_1	0.25_1
50	1.932_1	1.952_1	1.827_4	0.35_1	0.28_1
100	1.953_1	1.966_1	1.864_1	0.41_1	0.35_1

Subscript(s) indicate uncertainty in the last digit(s).

Table S13: Pure-component loading [in molecules/uc] in ACO at $T = 303$ K.

	Ethylene		Ethane		
p	UA	UA2	UA	UA2	EH
0.01	0.00071_1	0.00223_3		0.00018_1	
0.1	0.0070_1	0.0220_3	0.00226_4	0.00170_3	
0.2	0.0137_2	0.044_1	0.00448_3	0.00338_3	
0.5	0.034_1	0.114_2	0.0111_1	0.0083_1	0.00058_3
1	0.070_1	0.238_4	0.0220_4	0.0168_3	0.00113_3
1.5	0.105_2	0.38_1	0.0332_5	0.0252_3	0.0017_1
2	0.144_2	0.54_1	0.044_1	0.0332_5	0.0022_1
5	0.40_1	1.89_4	0.113_1	0.083_1	0.0056_3
10	0.97_2	4.17_4	0.234_4	0.164_2	0.011_1
20	3.2_1	5.15_2	0.50_1	0.325_6	0.020_1
30	4.59_3	5.41_1	0.80_3	0.48_1	0.028_1
40	5.03_2	5.54_1	1.13_3	0.60_2	0.034_1
50	5.24_1	5.61_1	1.49_4	0.67_1	0.038_1
100	5.516_1	5.718_5	2.2_1	0.83_2	0.045_1

Subscript(s) indicate uncertainty in the last digit(s).

Table S14: Pure-component loading [in molecules/uc] in UEI at $T = 303$ K.

	Ethylene		Ethane		
p	UA	UA2	UA	UA2	EH
0.001	0.00332_3	0.0046_1	0.0038_1		0.00269_3
0.01	0.0326_4	0.045_1	0.036_1	0.0090_1	0.0261_5
0.1	0.314_3	0.44_1	0.345_4	0.088_1	0.250_3
0.2	0.61_1	0.86_3	0.66_1	0.173_2	0.49_1
0.5	1.44_2	1.98_3	1.44_2	0.42_1	1.04_2
1	2.61_1	3.45_4	2.40_2	0.77_2	1.73_2
1.5	3.51_2	4.48_6	3.03_1	1.08_2	2.16_2
2	4.19_2	5.12_5	3.54_1	1.36_2	2.52_2
5	6.10_2	6.72_3	5.15_4	2.40_2	3.53_2
10	6.98_2	7.34_2	6.19_4	3.190_5	4.18_3
20	7.44_1	7.65_1	6.91_1	3.87_1	4.86_1
30	7.60_1	7.751_4	7.19_1	4.22_2	5.26_2
40	7.68_1	7.801_4	7.33_1	4.44_1	5.46_2
50	7.73_1	7.834_3	7.41_1	4.53_2	5.64_2
100	7.810_2	7.877_5	7.50_1	4.70_2	5.82_3

Subscript(s) indicate uncertainty in the last digit(s).

Table S15: Pure-component loading [in molecules/uc] in NAT at $T = 303$ K.

	Ethylene		Ethane		
p	UA	UA2	UA	UA2	EH
0.001				0.00172_3	0.00029_1
0.01	0.00353_5	0.00411_4	0.0040_1	0.0164_2	0.0029_1
0.1	0.0342_5	0.039_1	0.040_1	0.160_4	0.028_2
0.2	0.069_1	0.078_1	0.079_2	0.319_3	0.058_2
0.5	0.170_2	0.191_2	0.198_3	0.77_1	0.14_1
1	0.340_3	0.38_1	0.39_1	1.38_1	0.29_1
1.5	0.504_5	0.56_1	0.59_1	1.83_2	0.41_1
2	0.668_3	0.74_1	0.78_1	2.18_2	0.54_2
5	1.51_2	1.59_2	1.73_2	3.08_1	1.23_4
10	2.44_1	2.43_3	2.64_2	3.54_1	2.07_4
20	3.28_2	3.18_2	3.36_1	3.83_1	2.81_2
30	3.65_1	3.51_1	3.65_1	3.95_1	3.12_4
40	3.87_1	3.70_1	3.80_1	4.01_1	3.35_2
50	4.00_1	3.81_1	3.90_1	4.04_1	3.42_3
100	4.23_1	4.01_1	4.01_1	4.10_2	3.54_2

Subscript(s) indicate uncertainty in the last digit(s).

Table S16: Pure-component loading [in molecules/uc] in JRY at $T = 303$ K.

	Ethylene		Ethane		
p	UA	UA2	UA	UA2	EH
0.001	0.00120_2	0.00119_2	0.00162_2	0.0054_1	0.00111_2
0.01	0.0119_2	0.0120_2	0.0161_3	0.054_1	0.0116_4
0.1	0.118_2	0.118_2	0.158_2	0.49_1	0.112_4
0.2	0.229_4	0.229_1	0.309_3	0.87_1	0.23_1
0.5	0.541_5	0.52_1	0.71_1	1.58_1	0.54_2
1	0.98_1	0.93_1	1.24_1	2.13_1	0.99_3
1.5	1.33_1	1.24_1	1.61_1	2.40_1	1.27_2
2	1.60_1	1.47_1	1.88_1	2.58_1	1.52_2
5	2.49_1	2.21_1	2.67_1	3.01_1	2.33_3
10	3.02_2	2.66_1	3.08_1	3.27_1	2.82_3
20	3.38_1	2.99_1	3.38_2	3.45_1	3.15_2
30	3.54_1	3.132_4	3.50_1	3.55_2	3.31_3
40	3.62_1	3.21_1	3.57_1	3.60_2	3.40_3
50	3.66_1	3.27_1	3.61_2	3.61_1	3.42_3
100	3.75_1	3.37_1	3.66_1	3.66_1	3.46_3

Subscript(s) indicate uncertainty in the last digit(s).

Table S17: Pure-component loading [in molecules/uc] in ITW at $T = 303$ K.

	Ethylene			Ethane			
p	UA	UA2		UA	UA2		EH
		ITW-1	ITW-0		ITW-1	ITW-0	
0.001	0.00066_2	0.00329_4	0.00137_1	0.00079_1	0.00241_3	0.00273_3	0.00029_3
0.01	0.0063_1	0.032_1	0.0130_1	0.0076_1	0.0234_2	0.0276_4	0.0031_2
0.1	0.060_1	0.279_4	0.122_1	0.072_1	0.216_4	0.253_3	0.029_4
0.2	0.118_1	0.500_5	0.233_4	0.140_2	0.401_4	0.466_4	0.059_5
0.5	0.27_1	0.93_1	0.51_1	0.324_4	0.80_1	0.93_1	0.15_2
1	0.495_5	1.290_4	0.83_1	0.57_1	1.18_1	1.37_1	0.31_2
1.5	0.66_1	1.465_4	1.05_1	0.76_1	1.39_1	1.64_1	0.38_2
2	0.79_1	1.576_3	1.21_1	0.91_1	1.518_4	1.82_1	0.45_2
5	1.28_1	1.807_3	1.64_1	1.38_1	1.822_5	2.36_2	0.87_4
10	1.56_1	1.900_2	1.89_1	1.629_4	1.981_3	2.73_1	1.24_2
20	1.770_5	1.950_1	2.10_1	1.794_2	2.117_3	3.07_1	1.52_4
30	1.85_1	1.9680_4	2.22_1	1.851_1	2.19_1	3.25_2	1.63_2
40	1.896_4	1.9780_4	2.31_1	1.882_1	2.25_1	3.33_1	1.70_3
50	1.93_1	1.9838_3	2.379_4	1.900_1	2.26_1	3.38_2	1.74_1
100	1.989_2	1.996_1	2.53_1	1.919_1	2.31_1	3.43_1	1.78_1

Subscript(s) indicate uncertainty in the last digit(s).

Table S18: Pure-component loading [in molecules/uc] in RRO at $T = 303$ K.

	Ethylene			Ethane			
p	UA	UA2		UA	UA2		EH
		RRO-1	RRO-0		RRO-1	RRO-0	
0.001	0.00024_1	0.00031_1			0.00115_3		
0.01	0.0023_1	0.00292_5	0.00092_2	0.0025_1	0.0111_2	0.00312_5	0.0011_1
0.1	0.0218_5	0.0277_5	0.0087_1	0.0229_4	0.108_2	0.030_1	0.011_1
0.2	0.044_1	0.055_1	0.0171_2	0.046_1	0.207_4	0.060_1	0.024_4
0.5	0.106_2	0.134_2	0.042_1	0.111_1	0.48_1	0.144_2	0.054_6
1	0.207_3	0.257_3	0.082_1	0.214_5	0.82_1	0.276_4	0.12_1
1.5	0.30_1	0.366_5	0.121_2	0.31_1	1.07_2	0.396_5	0.15_1
2	0.39_1	0.47_1	0.156_4	0.40_1	1.24_1	0.50_1	0.20_1
5	0.82_1	0.90_1	0.35_1	0.83_1	1.77_1	0.977_3	0.46_4
10	1.25_1	1.31_1	0.597_5	1.24_1	2.10_1	1.37_1	0.81_5
20	1.68_1	1.67_1	0.92_1	1.63_1	2.33_1	1.74_1	1.17_4
30	1.89_1	1.845_4	1.11_1	1.80_2	2.43_1	1.90_1	1.41_5
40	2.02_1	1.94_1	1.231_5	1.91_1	2.51_1	1.99_1	1.51_2
50	2.09_1	2.01_1	1.31_1	1.97_1	2.53_1	2.04_1	1.57_4
100	2.24_1	2.14_1	1.48_1			2.11_1	1.69_3

Subscript(s) indicate uncertainty in the last digit(s).

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