Supplementary Information

Separating a linear C_5 hydrocarbon from a branched C_6 hydrocarbon : *n*-pentane from 2,2-dimethyl butane using Levitation and Blow torch effect

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TABLE S1. Potential energy parameters for modeling zeolite NaY.

Bonds	k_b (kJ.mol^{-1}.Å^{-2})	b_0 (Å)
Si-O	1260.0	1.61
Al-O	932.4	1.73
Angles	k_θ (kJ.mol^{-1}.rad^{-2})	θ_0 (^{o})
O-Si-O	337.5	109.5
O-Al-O	292.5	109.5
Si-O-Si	31.5	149.5
Al-O-Si	31.5	149.5
UB	k_u (kJ.mol^{-1}.Å^{-2})	u_0 (Å)
Si-(O)-Si	126.0	3.18
Al-(O)-Si	126.0	3.12
vDW Type	σ (Å)	ϵ (kJ.mol^{-1})
Si	3.92	2.52
Al	3.92	2.73
O	3.15	0.6384
Na	2.43	0.6678

TABLE S2. Lennard-Jones interaction parameters between zeolite NaY atoms and different groups of hydrocarbons of 2,2-dimethyl butane and n-pentane.

	σ (Å)	ϵ (kJ/mol)
Si-C	5.160	0.065
Si-CH_2	3.935	0.633
Si-CH_3	3.835	0.924
Al-C	5.160	0.067
Al-CH_2	3.935	0.658
Al-CH_3	3.835	0.961
O-C	4.475	0.051
O-CH_2	3.250	0.494
O-CH_3	3.150	0.722
Na-C	4.415	0.052
Na-CH_2	3.190	0.505
Na-CH_3	3.090	0.739

TABLE S3. Bonded and non-bonded interaction parameters of 2,2-dimethyl butane ($(H_3C\text{-})_3$(1,2,3)-C(4)-CH_2(5)-CH_3(6)) and *n*-pentane (CH_3(1)-CH_2(2)-CH_2(3)-CH_2(4)-CH_3(5)) molecules.

2,2-dimethyl butane				
	Angles	θ(°)	k_θ(kJ.mol^{-1}.rad^{-2})	
	6-5-4	114.0	519.625	
	5-4-1	109.5	519.625	
	5-4-2	109.5	519.625	
	5-4-3	109.5	519.625	
	2-4-1	109.5	519.625	
	2-4-3	109.5	519.625	
	1-4-3	109.5	519.625	
Dihedrals	c_0	c_1	c_2	c_3
ϕ	(K*k_B)	(K*k_B)	(K*k_B)	(K*k_B)
6-5-4-1	0.00	0.00	0.00	3.835
6-5-4-2	0.00	0.00	0.00	3.835
6-5-4-3	0.00	0.00	0.00	3.835
n-pentane				
	Angles	θ(°)	k_θ(kJ.mol^{-1}.rad^{-2})	
	1-2-3(3)	114.0	519.625	
Dihedrals	c_0	c_1	c_2	c_3
ϕ	(K*k_B)	(K*k_B)	(K*k_B)	(K*k_B)
1-2-3-4(2)	0.00	2.95	-0.56	6.58
Nonbonded(self interaction)				
	Group	σ Å	ϵ (kJ/mol)	
	C-C	6.400	0.004	
	CH_2-CH_2	3.950	0.382	
	CH_3-CH_3	3.750	0.814	