Supporting Information for

Encapsulation of Highly Volatile Fragrances in Y Zeolites for Sustained Release: Experimental and Theoretical Studies

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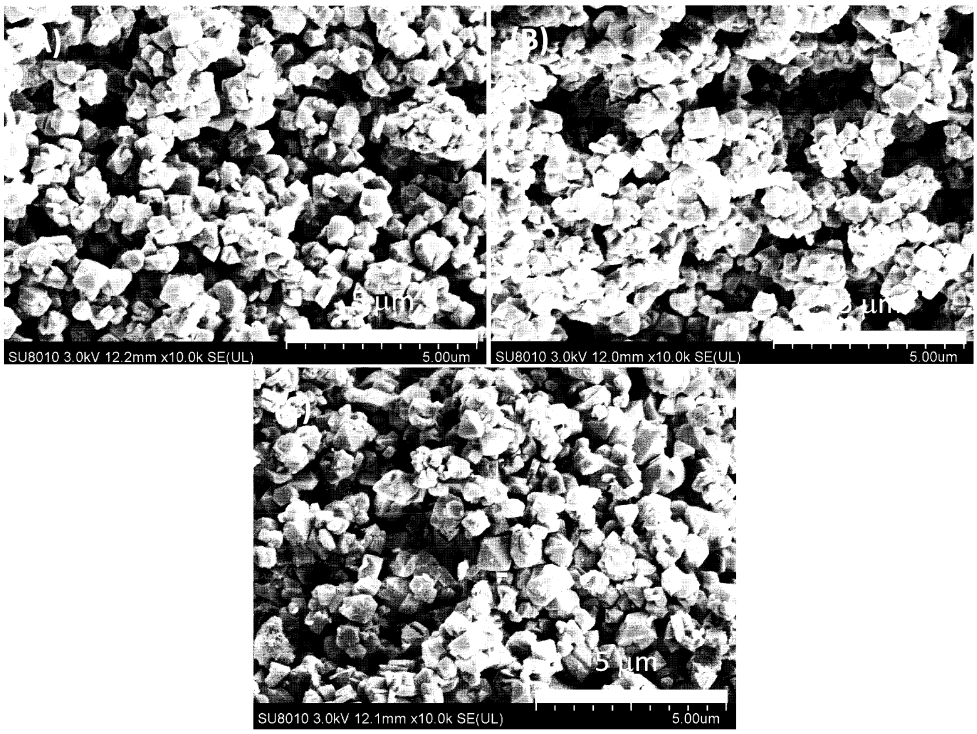

Figure S1. SEM images of Y-type zeolites with different extra-framework metal ions: (A) NaY, (B) $Ca_{0.91}Y$, and (C) $La_{0.90}Y$. The latter two were obtained from the parent zeolite NaY by an ion-exchanging process.

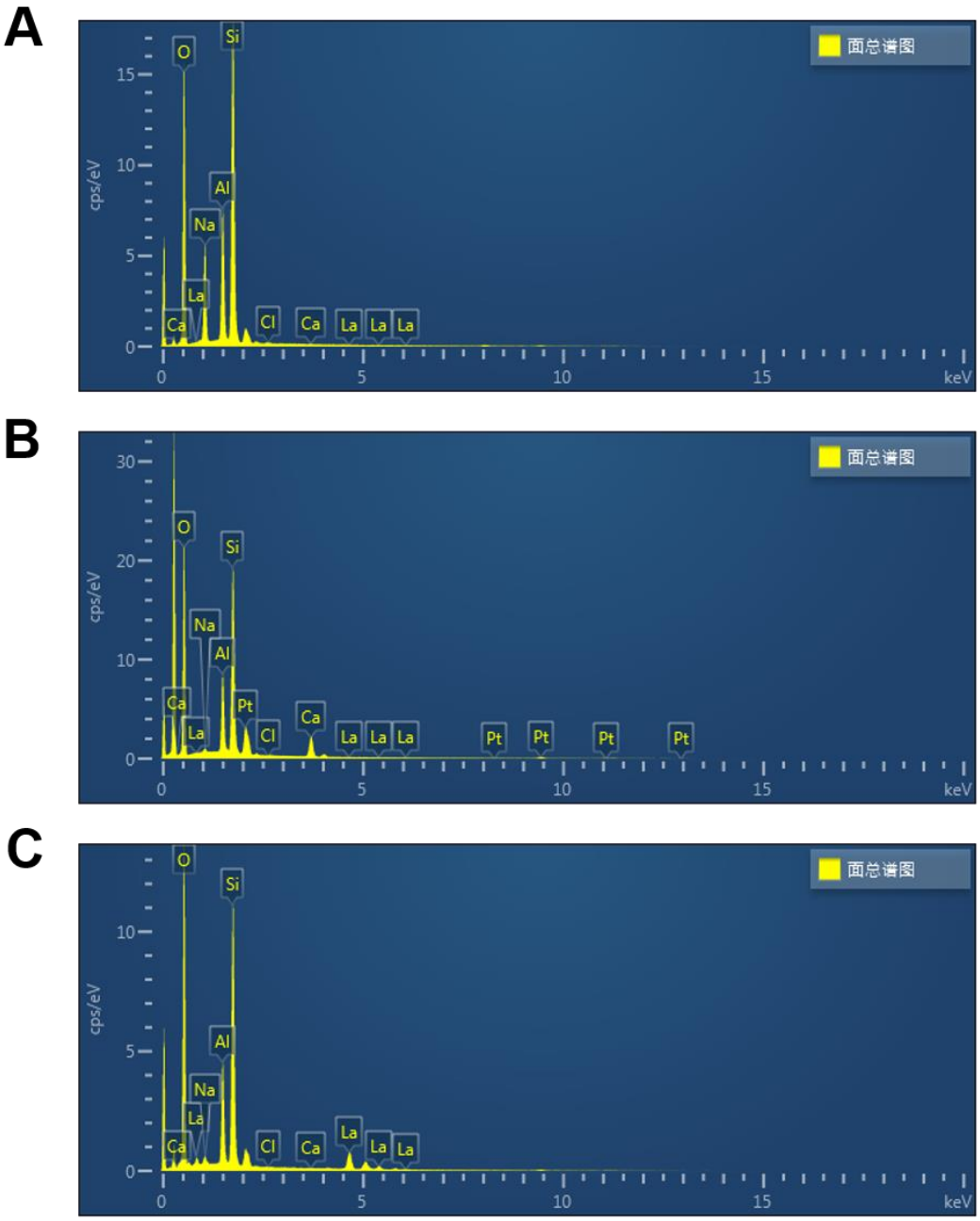

Figure S2. Total energy dispersion spectra on the surface of Y zeolites with different extra-framework cations: (A) NaY; (B) $Ca_{0.91}Y$; (C) $La_{0.90}Y$.

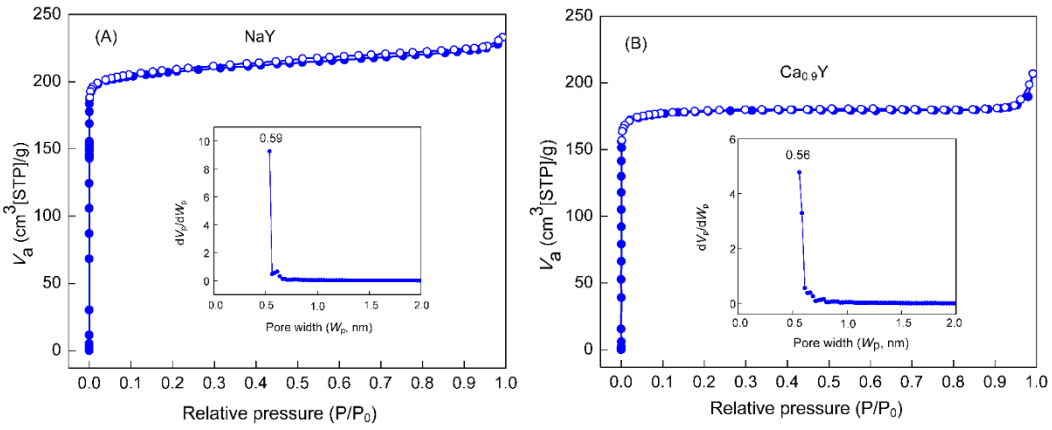

Figure S3. N_2 adsorption−desorption isotherms measured at 77 K for $Ca_{0.91}Y$ (A) and $La_{0.90}Y$ (B). Insets: the corresponding pore width distribution curve derived from desorption isotherm branches by the BJH method.

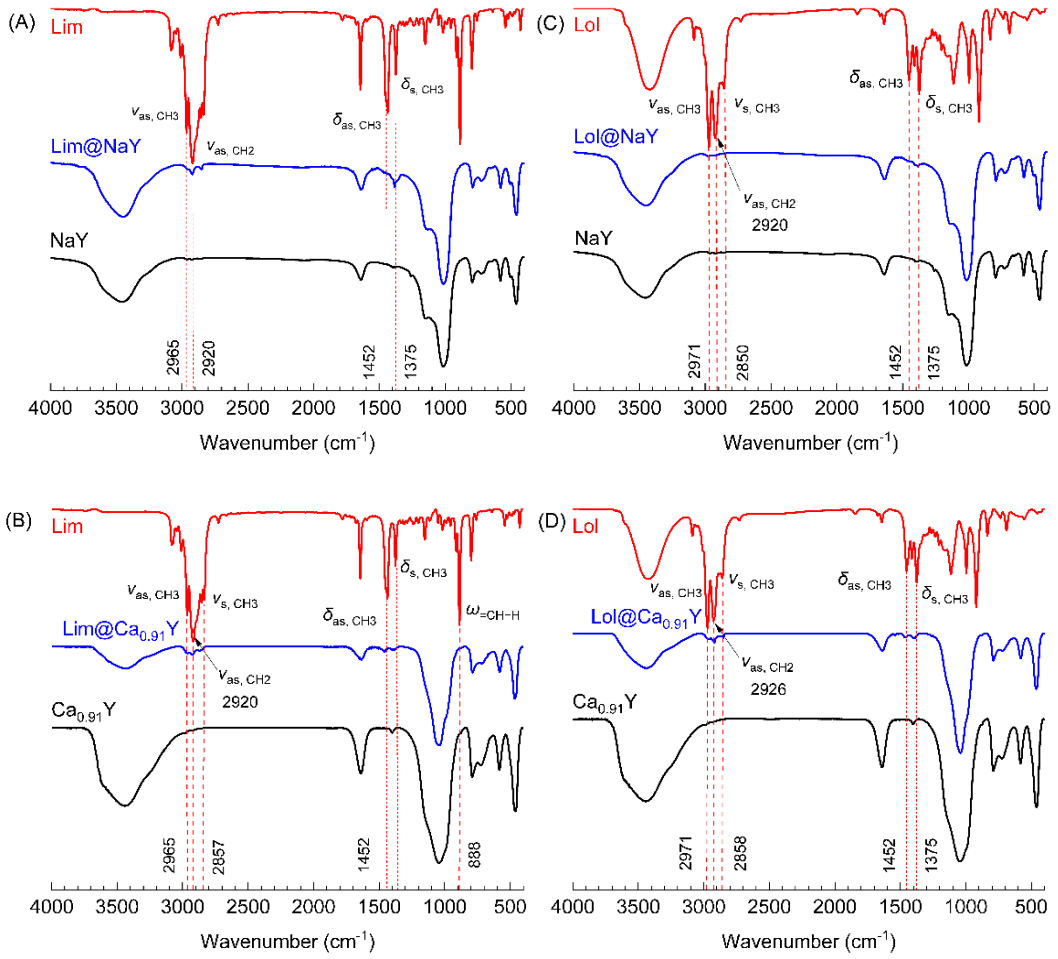

Figure S4. Comparison of IR spectra of neat fragrances limonene (A, B) and linalool (C, D) with that of Y zeolites and composites FG@ZY thereof.

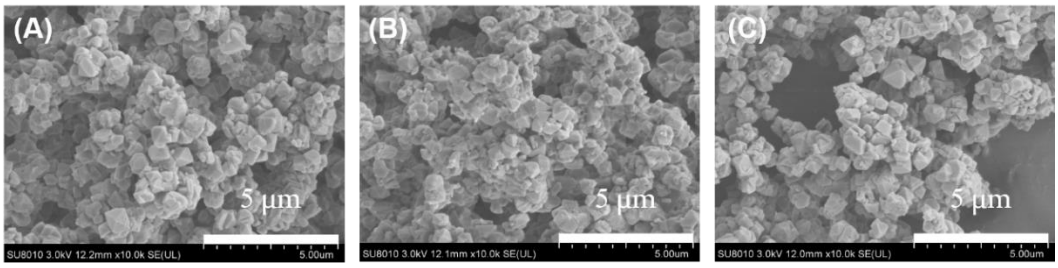

Figure S5. SEM images of linalool-loaded composites: (A) Lol@NaY, (B) Lol@$Ca_{0.91}$Y, and (C) Lol@$La_{0.90}$Y.

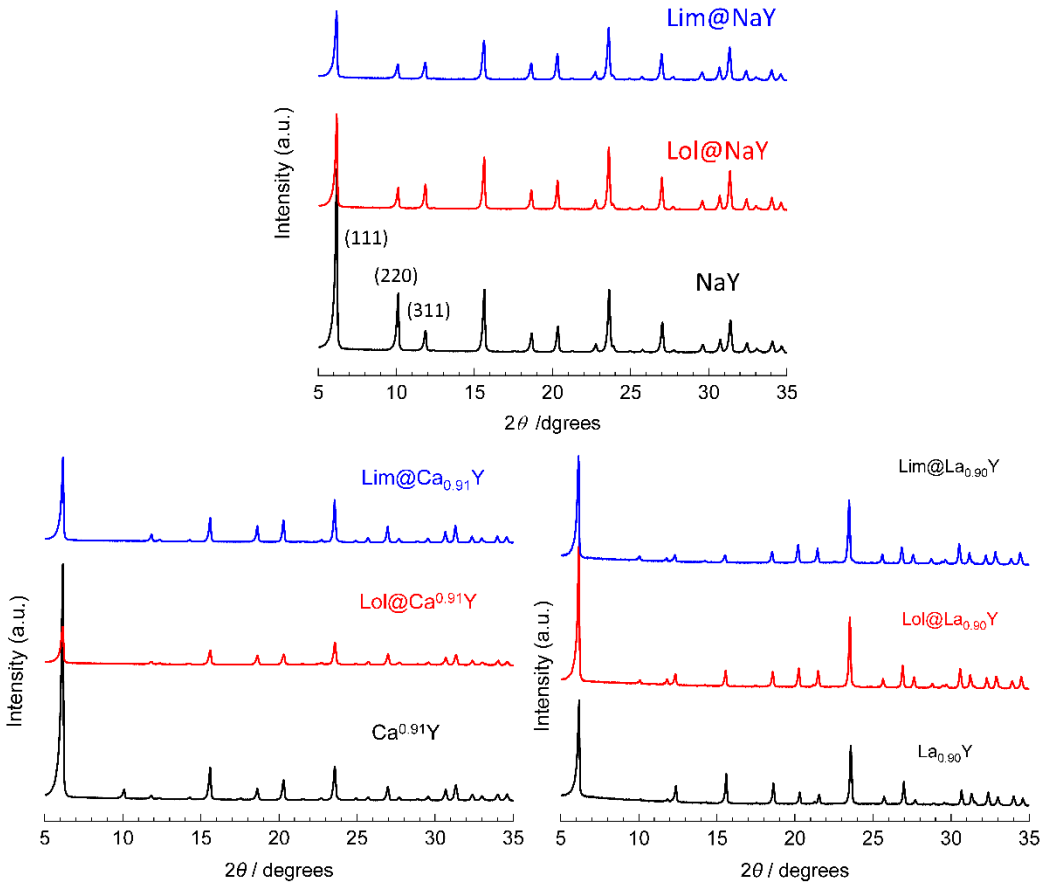

Figure S6. Comparison of powder X-ray diffraction (PXRD) patterns of Y zeolites with the corresponding fragrance-loaded composites.

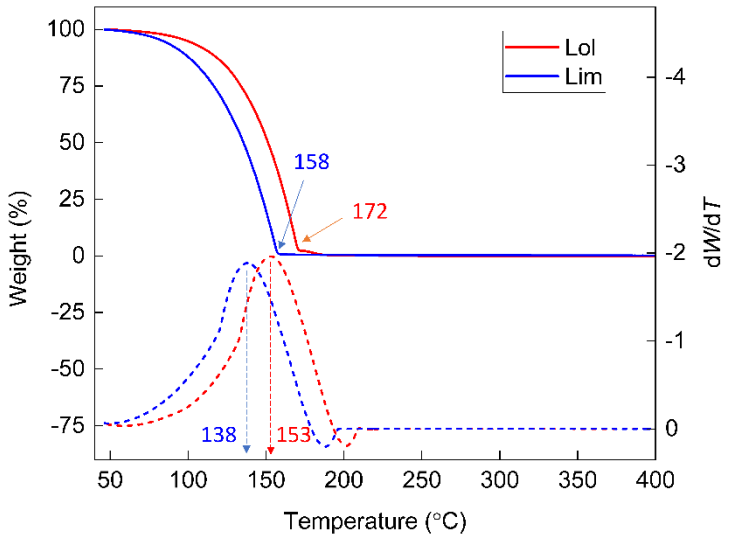

Figure S7. TGA curves of free fragrances D-limonene and linalool.

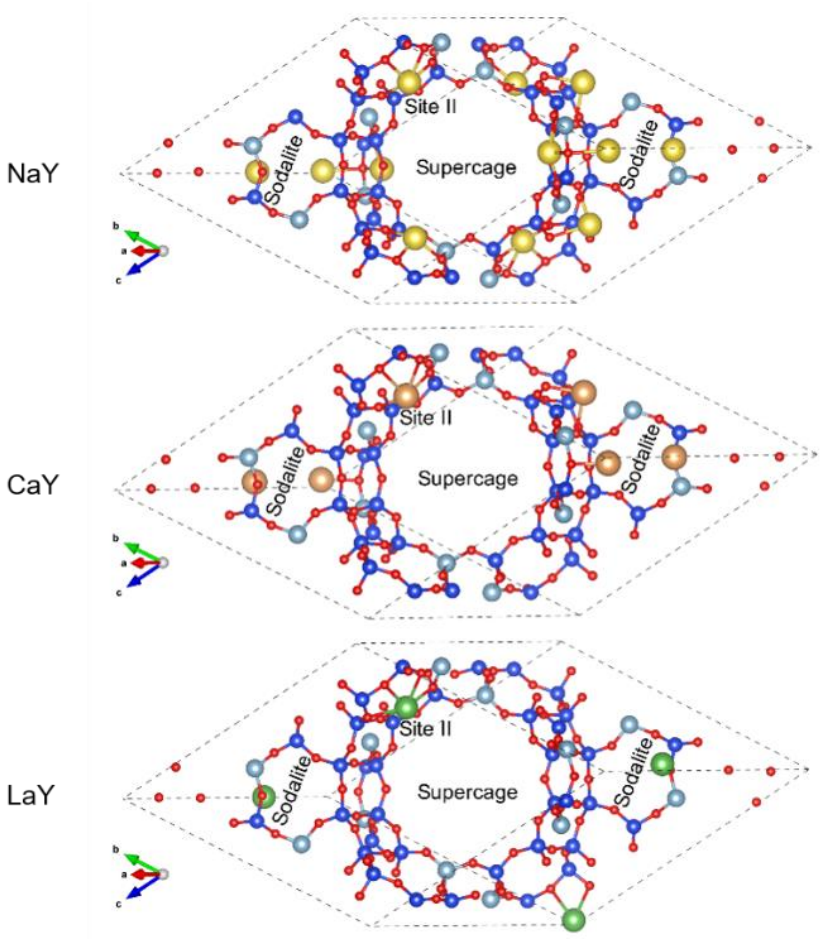

Figure S8. Periodic model of a primitive cell of the zeolite NaY, CaY, and LaY (Si: blue; Al: grey; O: red; Na: yellow; Ca: brown; La: green).

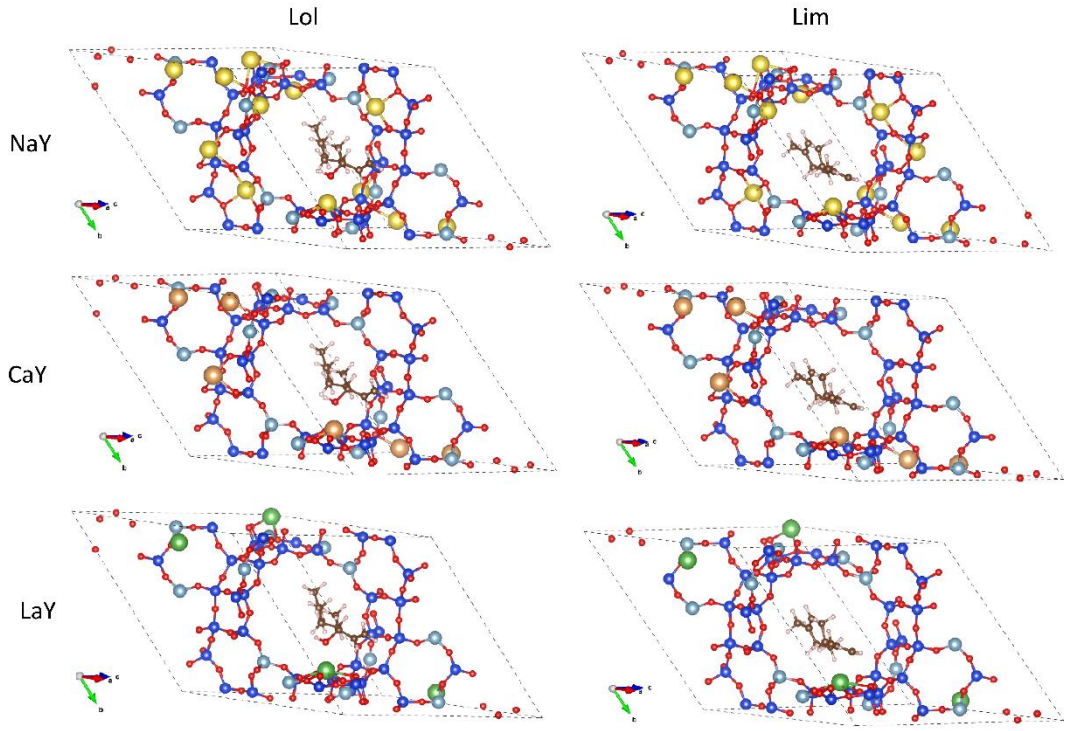

Figure S9. The most stable adsorption configurations of fragrance molecules onto Y zeolites NaY, CaY, and LaY at a primitive cell scale.

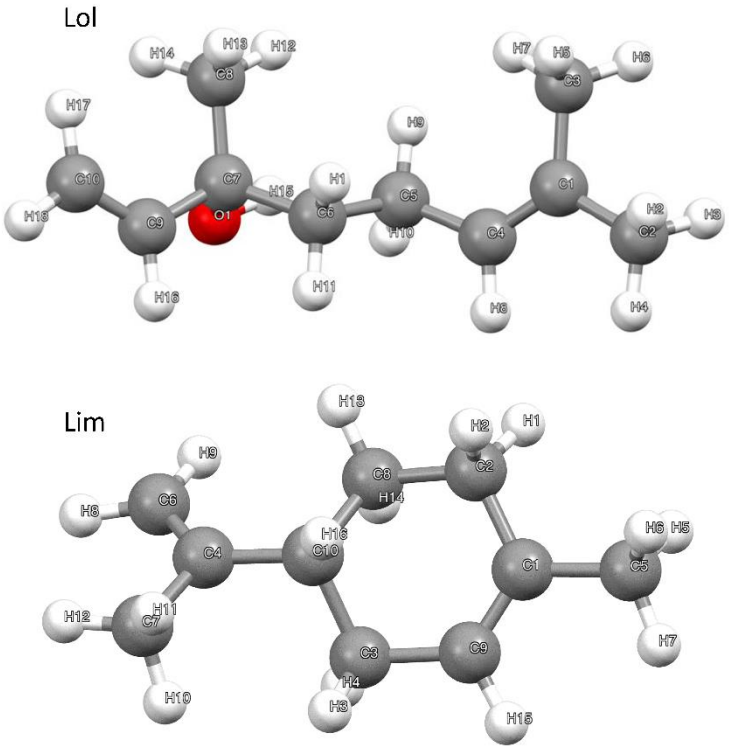

Figure S10. The chemical structures of linalool (Lol) and limonene (Lim) with labels on the atoms.

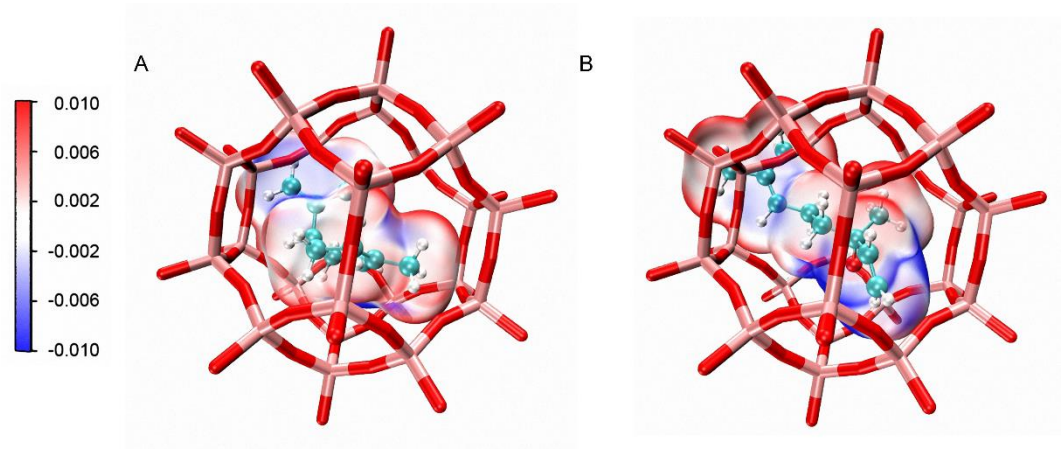

Figure S11. Graphical representation of the shape-selectivity of the sodalite cage in Y zeolites towards D-limonene (A) and linalool (B).

Table S1. Preparation of La_xY starting from $La_{0.62}Y$ [a]

Calcination-impregnation cycles	0	1	2	3
Ion exchange degree, *x*	0.62	0.90	0.95	0.97

[a] Calcination for 6 h at 400 °C followed by soaking with 1.0 M $LaCl_3$ solution for 24 h at r.t. is considered a cycle.

Table S2. Chemical composition of Y-type zeolites determined by energy dispersive spectroscopy

Element	Element content (wt-%)		
	NaY	$Ca_{0.91}Y$	$La_{0.90}Y$
O	64.70	76.08	73.11
Na	8.51	0.48	0.73
Al	7.64	6.14	6.83
Si	19.15	14.71	17.12
Cl	0.00	0.00	0.00
Ca	0.00	2.59	0.00
La	0.00	0.00	2.21
Total	100.00	100.00	100.00

Table S3. Fragrance release kinetic parameters for FG@NaY composites

Sample	First-order Eq.		Higuchi Eq.		Weibull Eq.		
	k (s^{-1})	R^2	k ($s^{-0.5}$)	R^2	k (s^{-1})	n	R^2
Lol@NaY	1.9×10^{-7}	0.9249	4.4×10^{-3}	0.9815	1.7×10^{-7}	0.40	0.9845
Lim@NaY	1.1×10^{-7}	0.9878	3.6×10^{-3}	0.9997	6.1×10^{-8}	0.38	0.9993

Table S4. Zero-order kinetic parameters for the release of fragrance from FG@$Ca_{0.91}Y$ and FG@$La_{0.90}Y$

Sample	Lol@$Ca_{0.91}Y$	Lim@$Ca_{0.91}Y$	Lol@$La_{0.90}Y$	Lim@$La_{0.90}Y$
k (s^{-1})	1.0×10^{-7}	4.7×10^{-8}	8.6×10^{-8}	3.7×10^{-8}
R^2	0.9996	0.9914	0.9930	0.9947

Table S5. The Bader charge differences of linalool in Y-type zeolites (see Figure S10)

ΔQ	Lol		
	NaY	CaY	LaY
O1	0.4820	0.4870	0.4660
C1	–0.0198	0.0226	0.0116
C2	0.0074	–0.0095	–0.0025
C3	–0.0625	–0.0041	0.0114
C4	–0.0078	–0.0078	–0.0081
C5	–0.0520	–0.0115	–0.0032
C6	–0.0035	–0.0080	0.0041
C7	–0.0064	–0.0396	–0.0585
C8	0.0017	–0.0033	–0.0206
C9	–0.0174	–0.0211	–0.0702
C10	0.0112	0.0184	0.0402
H1	–0.0009	0.0274	0.0544
H2	0.0249	0.0294	0.0128
H3	–0.0166	0.0055	0.0054
H4	–0.0131	–0.0043	0.0051
H5	0.1150	0.0158	0.0169
H6	0.0070	0.0268	0.0294
H7	–0.0192	–0.0183	–0.0132
H8	0.0070	0.0130	0.0130
H9	0.0543	0.0089	0.0108
H10	0.0064	–0.0122	–0.0266
H11	0.0036	0.0089	0.0167
H12	0.0079	0.0172	0.0369
H13	0.0034	0.0275	0.0471
H14	0.0089	0.0063	0.0095
H15	0.0239	0.0465	0.0589
H16	0.0053	0.0062	0.0121
H17	0.0066	0.0197	0.0314
H18	0.0098	0.0311	0.0447
Total	0.5670	0.6780	0.7350

Table S6. The Bader charge differences of limonene in Y-type zeolites (see Figure S10).

ΔQ	Lim		
	NaY	CaY	LaY
C1	0.0118	0.0100	0.0197
C2	–0.0026	–0.0055	–0.1120
C3	0.0011	0.0129	–0.0452
C4	–0.0188	–0.0569	–0.0636
C5	0.0007	0.0134	0.0206
C6	–0.0909	–0.0971	–0.1820
C7	–0.0342	–0.0393	–0.0998
C8	–0.0143	–0.0107	0.0060
C9	0.0021	0.0182	0.0310
C10	–0.0101	–0.0220	–0.0166
H1	–0.0063	0.0166	0.0149
H2	0.0393	0.0298	0.1300
H3	–0.0046	0.0033	0.0112
H4	–0.0062	0.0016	0.0032
H5	–0.0068	0.0034	–0.0121
H6	–0.0035	–0.0022	0.0175
H7	0.0092	0.0216	0.0230
H8	0.0017	0.0118	0.0256
H9	0.0659	0.0439	0.1400
H10	0.0391	0.0597	0.1280
H11	0.0226	0.0226	0.0215
H12	–0.0066	–0.0079	–0.0033
H13	0.0142	0.0060	0.0010
H14	0.0053	0.0083	0.0209
H15	–0.0063	0.0187	0.0336
H16	0.0250	0.0220	0.0459
Total	0.0268	0.0824	0.1590