Supporting Information

Oxidative Dehydrogenation of Propane to Propylene in the Presence of HCl Catalyzed by CeO_2 and NiO-Modified CeO_2 Nanocrystals

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1. Syntheses of CeO_2 Nanocrystals with Different Morphologies

CeO_2 nanocrystals with different morphologies were synthesized by hydrolysis of Ce(III) salts in alkaline medium, followed by a hydrothermal treatment.[1,2] For the synthesis of CeO_2 nanorods, 0.69 g $Ce(NO_3)_3 \cdot 6H_2O$ and 50.4 g NaOH were first dissolved in 20 and 140 cm^3 deionized water, respectively. Then, the two aqueous solutions were mixed together in a Teflon bottle and the mixture was kept stirring for 6 h, forming a milky suspension. Subsequently, the Teflon bottle containing this suspension was placed in a stainless-steel autoclave and was subjected to hydrothermal treatment at 373 K for 24 h. The same procedure was adopted for the synthesis of CeO_2 nanocubes and nanoparticles except for the amount of NaOH and the hydrothermal temperature employed. The amount of NaOH was 33.6 g and the hydrothermal temperature was 453 K for nanocubes, while they were 0.50 g and 373 K for nanoparticles. For the synthesis of CeO_2 nano-octahedra, 1.74 g $Ce(NO_3)_3 \cdot 6H_2O$ and 0.015 g $Na_3PO_4 \cdot 12H_2O$ were dissolved in 140 cm^3 deionized water. After being stirred at room temperature for 3 h, the mixed solution was transferred into a Teflon-lined stainless-steel autoclave and was subjected to hydrothermal treatment at 473 K for 24 h. After the hydrothermal treatment in each case, the solid product was recovered by centrifugation, followed by washing with deionized water and ethanol repeatedly for several times, and drying at 373 K in air overnight. Finally, the solid sample was calcined at 823 K in air for 6 h.

2. Supplementary Tables and Figures

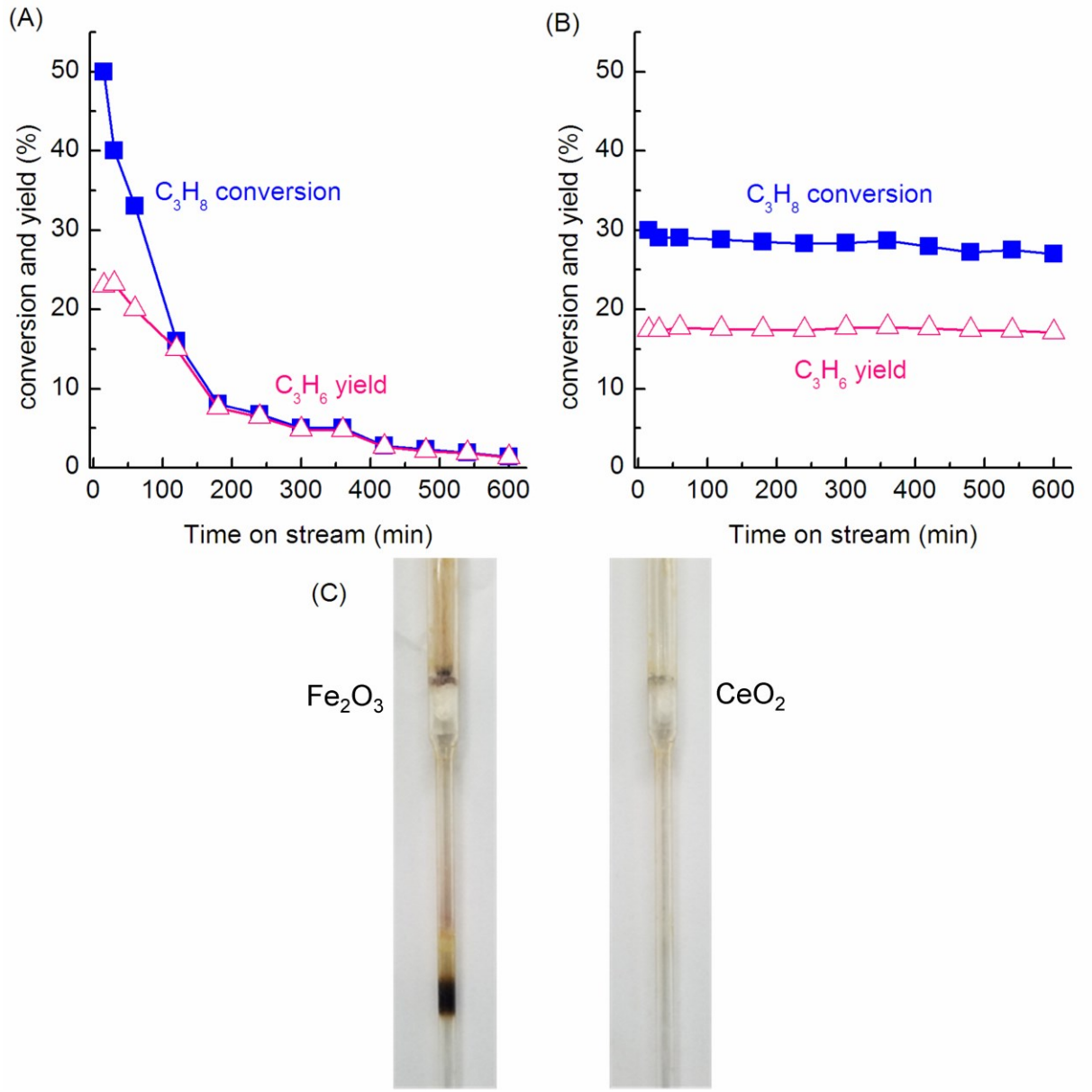

Figure S1. Comparison of stability of Fe_2O_3 and CeO_2 in the conversion of C_3H_8 by (O_2 + HCl). (A) Fe_2O_3. (B) CeO_2. (C) Reactors for Fe_2O_3 and CeO_2 catalysts after reactions. Reaction conditions: catalyst, 0.10 g; $P(C_3H_8)$ =18 kPa; $P(O_2)$ =18 kPa; P(HCl) =10 kPa; F = 48 mL min^{-1}; T = 773 K. The dark brown solid in the downstream of the reactor was observed after the reaction for 10 h for Fe_2O_3 but not for CeO_2.

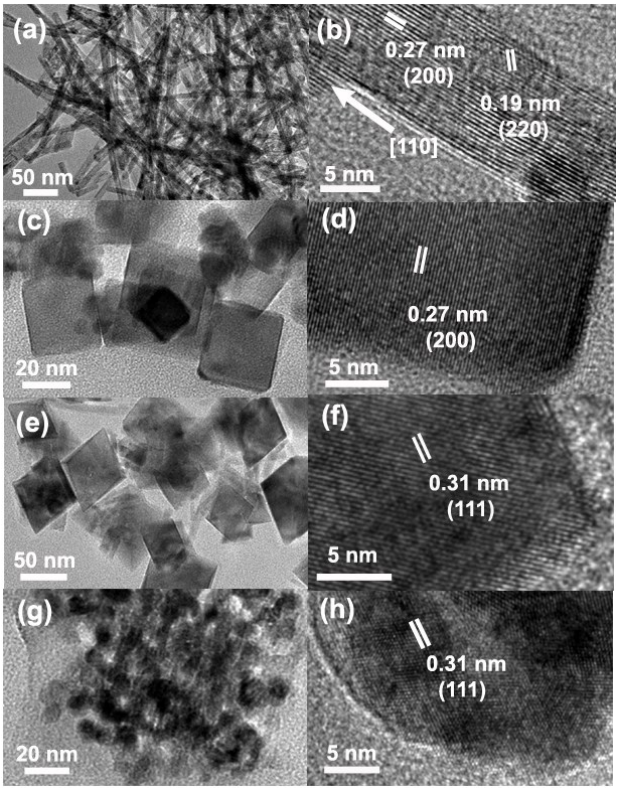

Figure S2. TEM and HRTEM micrographs for CeO_2 nanocrystals with different morphologies. Nanorod: (a) TEM, (b) HRTEM. Nanocube: (c) TEM, (d) HRTEM. Nano-octahedron: (e) TEM, (f) HRTEM. Nanoparticle: (g) TEM, (h) HRTEM.

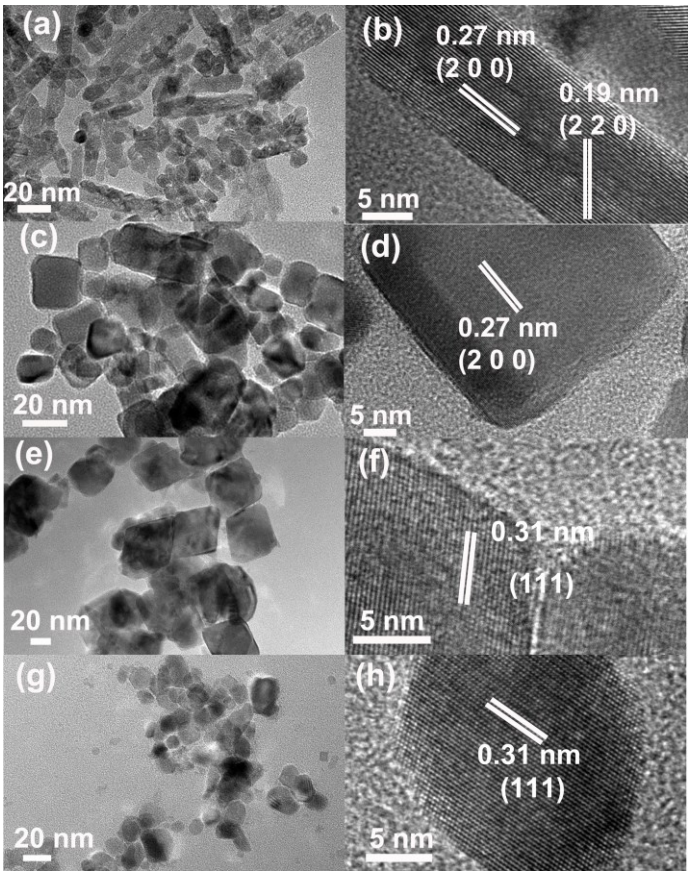

Figure S3. TEM and HRTEM micrographs for CeO_2 nanocrystals with different morphologies after the conversion of C_3H_8 by (O_2 + HCl) for 10 h. Nanorod: (a) TEM, (b) HRTEM. Nanocube: (c) TEM, (d) HRTEM. Nano-octahedron: (e) TEM, (f) HRTEM. Nanoparticle: (g) TEM, (h) HRTEM.

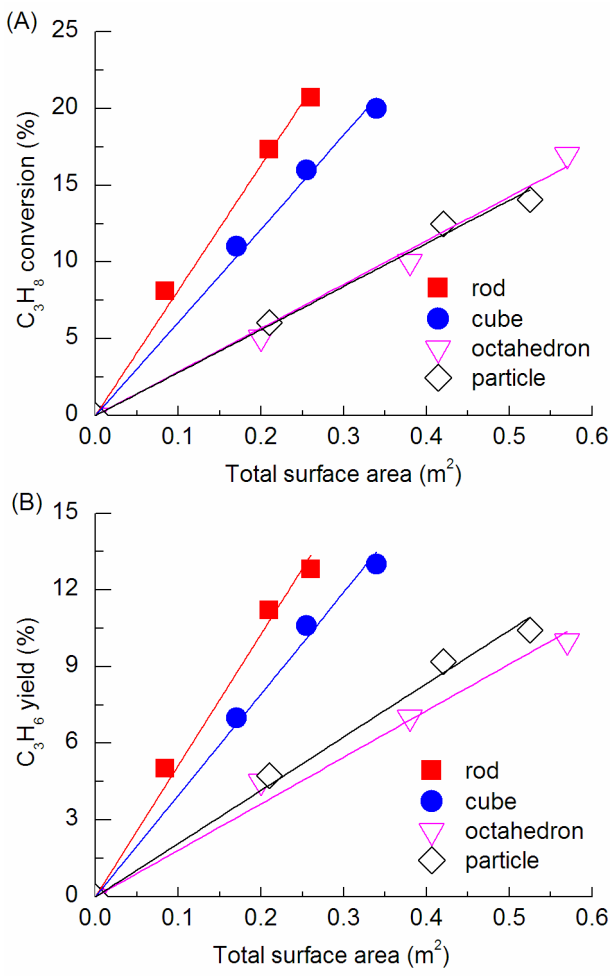

Figure S4. Catalytic performances of CeO_2 nanocrystals with different morphologies. (A) C_3H_8 conversion versus total catalyst surface area. (B) C_3H_6 yield versus total catalyst surface area. Reaction conditions: catalyst 0.005-0.10 g; $P(C_3H_8)$ = 18 kPa; $P(O_2)$ = 18 kPa; P(HCl) = 10 kPa; F = 48 mL min^{-1}; T = 773 K; time on stream, 3 h.

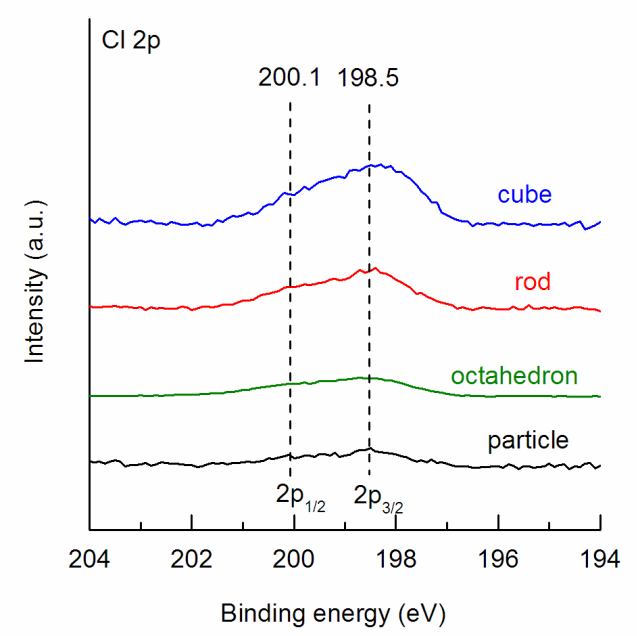

Figure S5. Cl 2p XPS spectra for CeO_2 nanocrystals with different morphologies after HCl chemisorption at 773 K.

Table S1. Catalytic Performances of Modified CeO_2 Nanorods for the Conversion of C_3H_8 by (O_2 + HCl)[a]

catalyst[b]	conversion (%)		selectivity (%)						C_3H_6 yield (%)
	C_3H_8	O_2	C_3H_6	C_3H_7Cl	C_3H_5Cl	C_2H_6	CO	CO_2	
CeO_2 rod	38	77	55	0.6	1.8	2.1	19	20	21
V_2O_5−CeO_2	34	60	68	1.7	1.0	1.8	11	16	23
MoO_3−CeO_2	25	25	80	1.5	2.1	1.7	8.5	5.5	20
MgO−CeO_2	49	80	62	1.0	0.9	6.0	12	18	30
MnO−CeO_2	55	81	61	1.0	0.6	10	11	14	34
Fe_2O_3−CeO_2	44	83	51	0.6	3.1	1.2	21	23	22
Co_3O_4−CeO_2	33	62	62	1.3	2.0	3.2	12	17	20
NiO−CeO_2	52	65	72	2.2	1.2	1.8	7.6	15	37
CuO−CeO_2	40	93	56	0.5	1.0	0.9	13	27	22
ZnO−CeO_2	43	80	58	0.8	1.6	2.8	17	18	25

[a] Reaction conditions: catalyst, 0.10 g; $P(C_3H_8)$ = 18 kPa; $P(O_2)$ = 18 kPa; P(HCl) = 10 kPa; F = 48 mL min^{-1}; T = 773K; time on stream, 3 h. [b] The content of metal oxide modifier, 8 wt%.

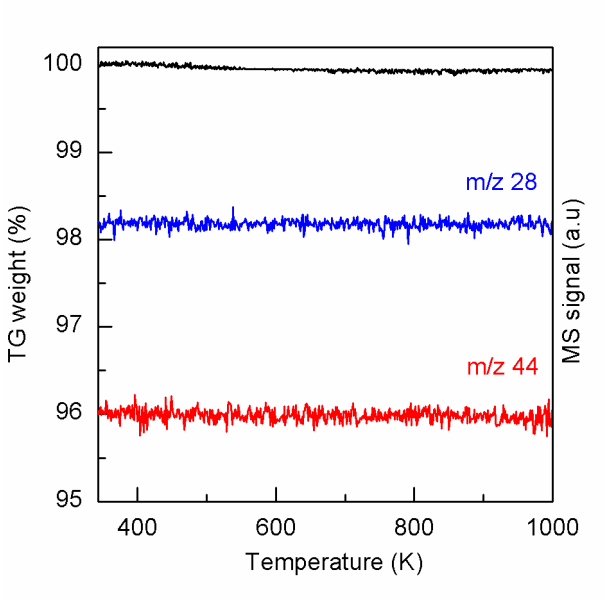

Figure S6. Thermogravimetric analysis (black line, left axis) and O_2-TPO profiles (blue and red lines, right axis) for the 8 wt% NiO−CeO_2 catalyst after 100 h of reaction.

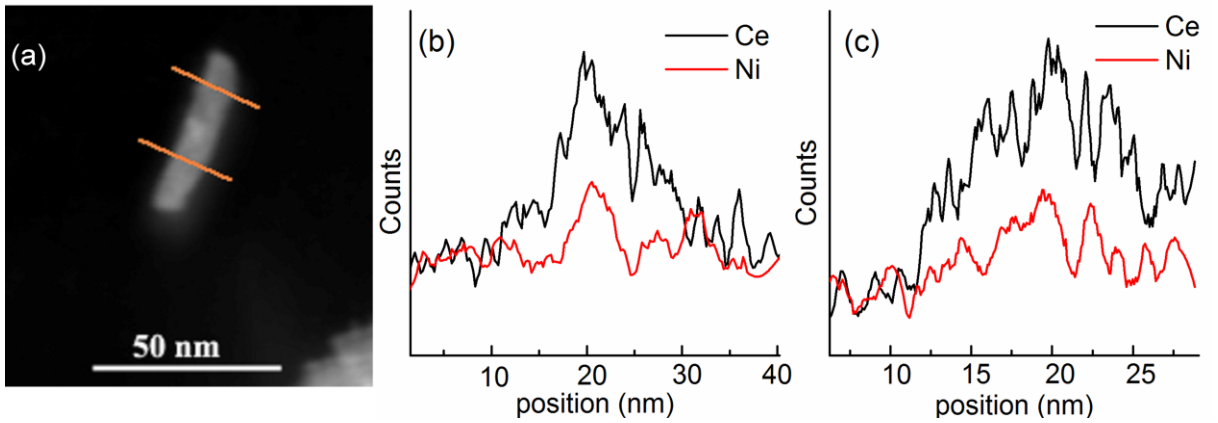

Figure S7. (a) Representative TEM micrograph (dark field) for 8 wt% NiO−CeO_2 catalyst. (b) and (c) Line-scan EDS analyses across the rod in two places (two lines in the TEM micrograph).

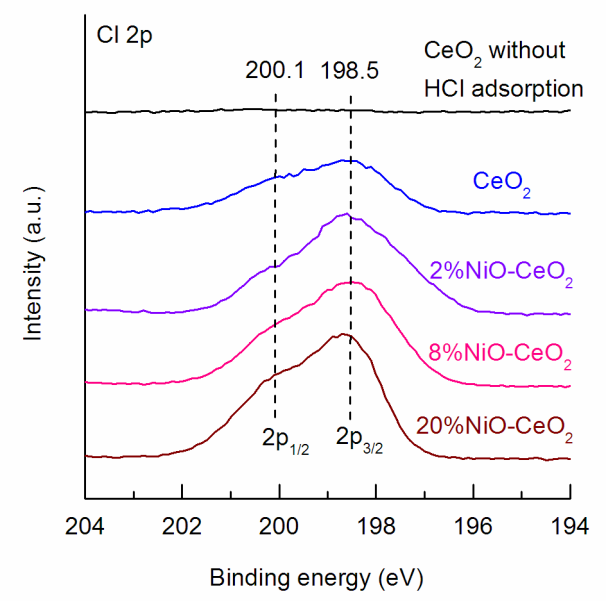

Figure S8. Cl 2p XPS spectra for NiO−CeO_2 catalysts with different NiO contents after HCl chemisorption at 773 K. The result for CeO_2 without HCl chemisorption was also displayed as a reference.

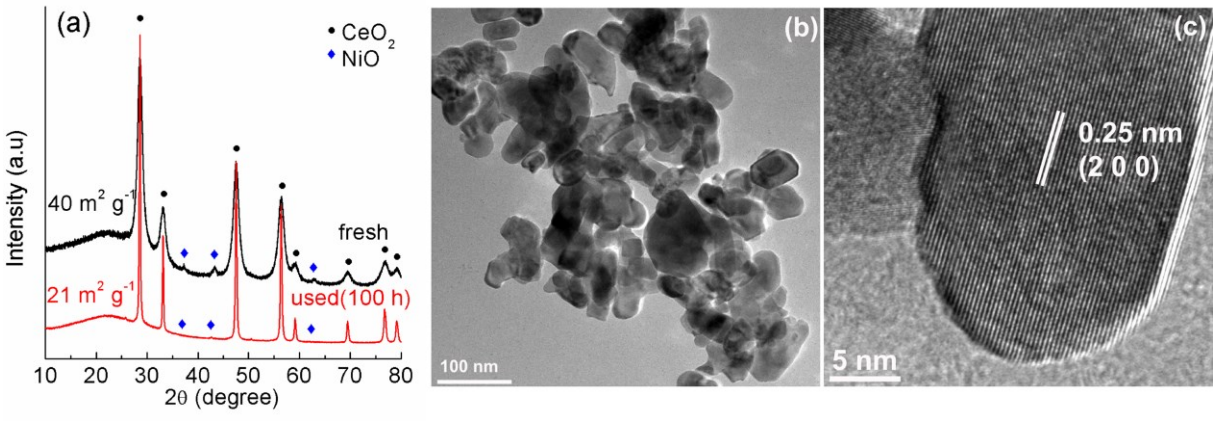

Figure S9. Characterization results for the 8 wt% NiO−CeO_2 catalyst after 100 h of reaction. (a) XRD patterns and total surface area including the fresh catalyst. (b) TEM micrograph. (c) HRTEM micrograph.

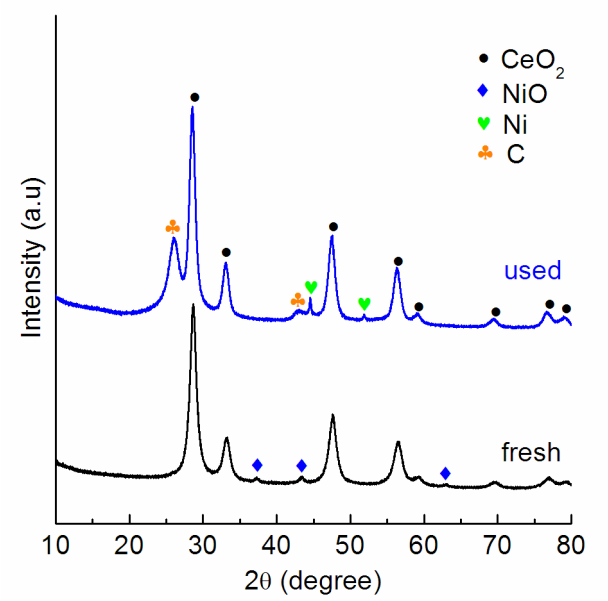

Figure S10. XRD patterns for the 8 wt% NiO−CeO_2 catalyst before and after the (C_3H_8 + O_2) reaction under conditions in Figure 7B with *P*(HCl) = 0.

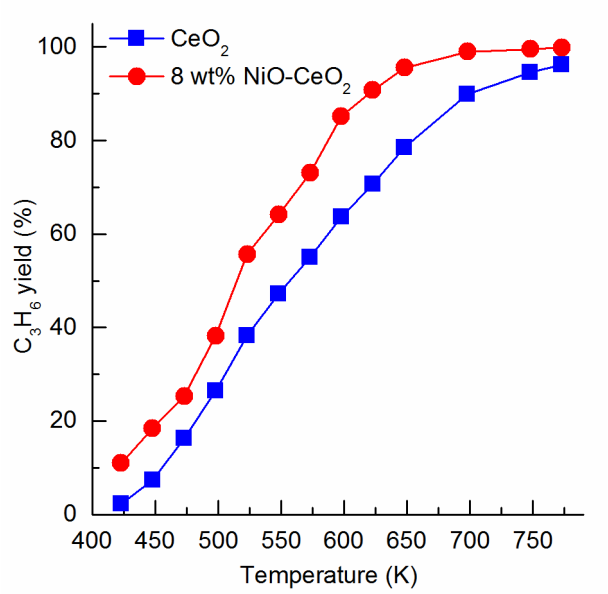

Figure S11. Yields of C_3H_6 versus temperature in the dehydrochlorination of C_3H_7Cl over CeO_2 and 8 wt% NiO−CeO_2 catalysts. Reaction conditions: catalyst, 0.10 g; F(C_3H_7Cl, liquid) = 0.30 cm^3 h^{-1}; P(N_2) = 15 kPa; P(He) = 86 kPa; F = 48 mL min^{-1}; time on stream, 3 h.

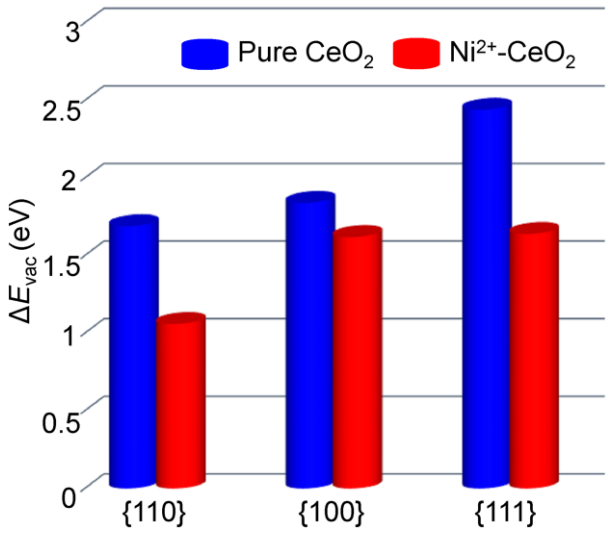

Figure S12. Formation energy of oxygen vacancies (ΔE_{vac}) on different facets of CeO_2 and the corresponding facets modified by Ni^{2+} cations.

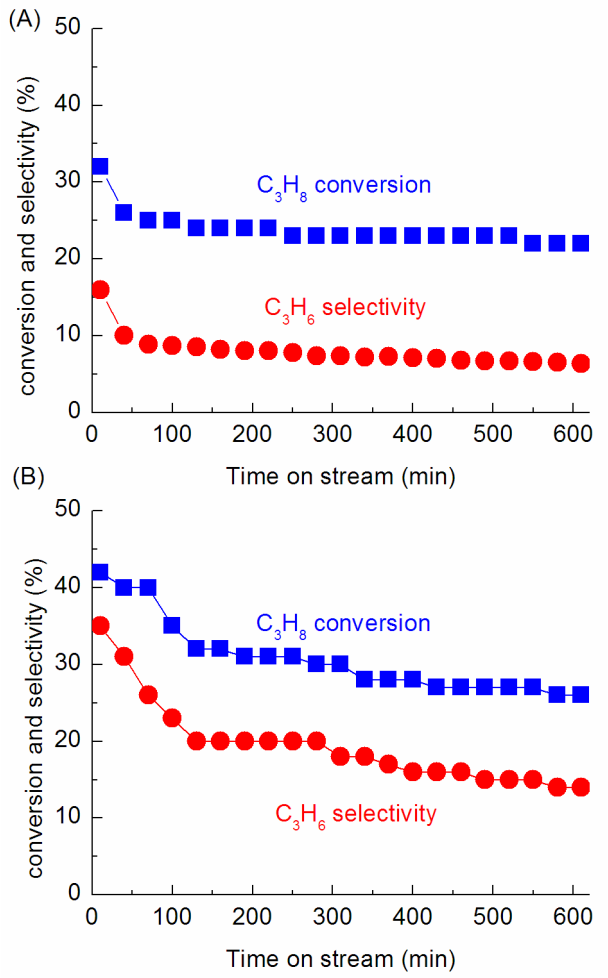

Figure S13. Conversion of C_3H_8 by O_2 over catalysts with HCl pre-chemisorbed. (A) CeO_2. (B) 8 wt% NiO−CeO_2. Reaction conditions: catalyst 0.10 g; $P(C_3H_8)$ = 18 kPa; $P(O_2)$ = 18 kPa; F = 48 mL min^{-1}; T = 773 K.

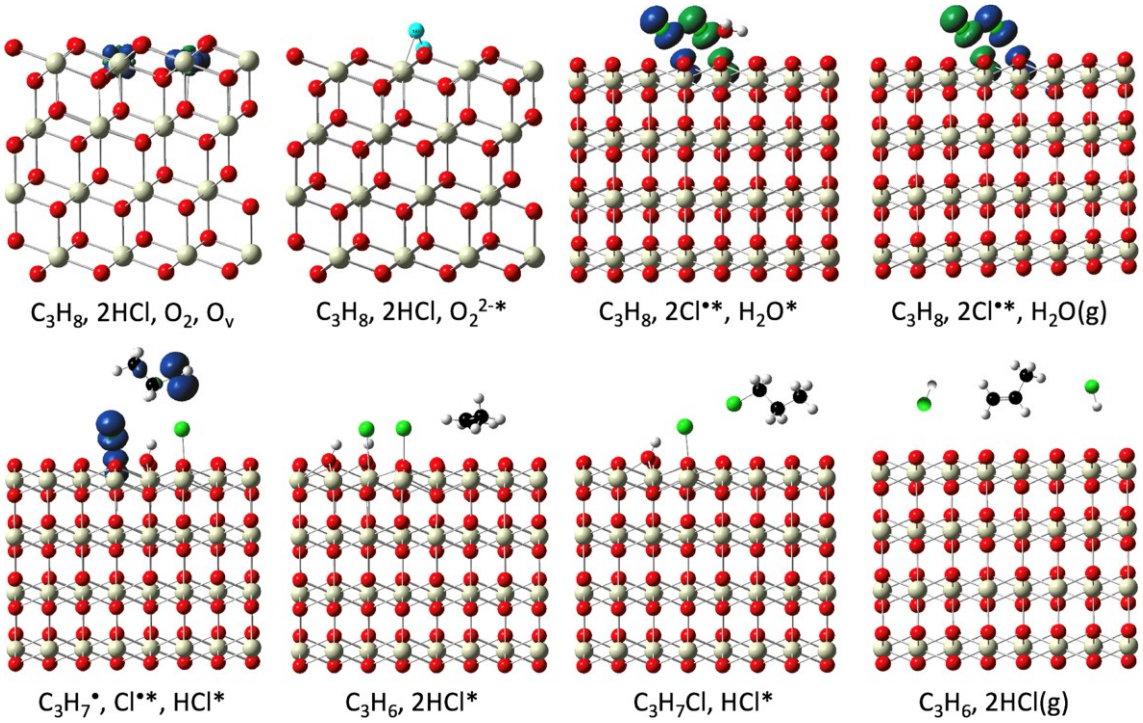

Figure S14. Configurations of the key intermediates in Figure 12.

H is white; C is black; O is red; Ce is ivory; Cl is green. The dark green and blue area are spin density isosurface of unpaired electron in Ce^{3+} or Cl radicals with isovalue of 0.005 e/Å^3. The absorbed species on surfaces of CeO_2 and the gas-phase products (C_3H_7•, C_3H_7Cl, C_3H_6, HCl) are mainly presented, while gas-phase reactants (C_3H_8, O_2 and HCl) are neglected.

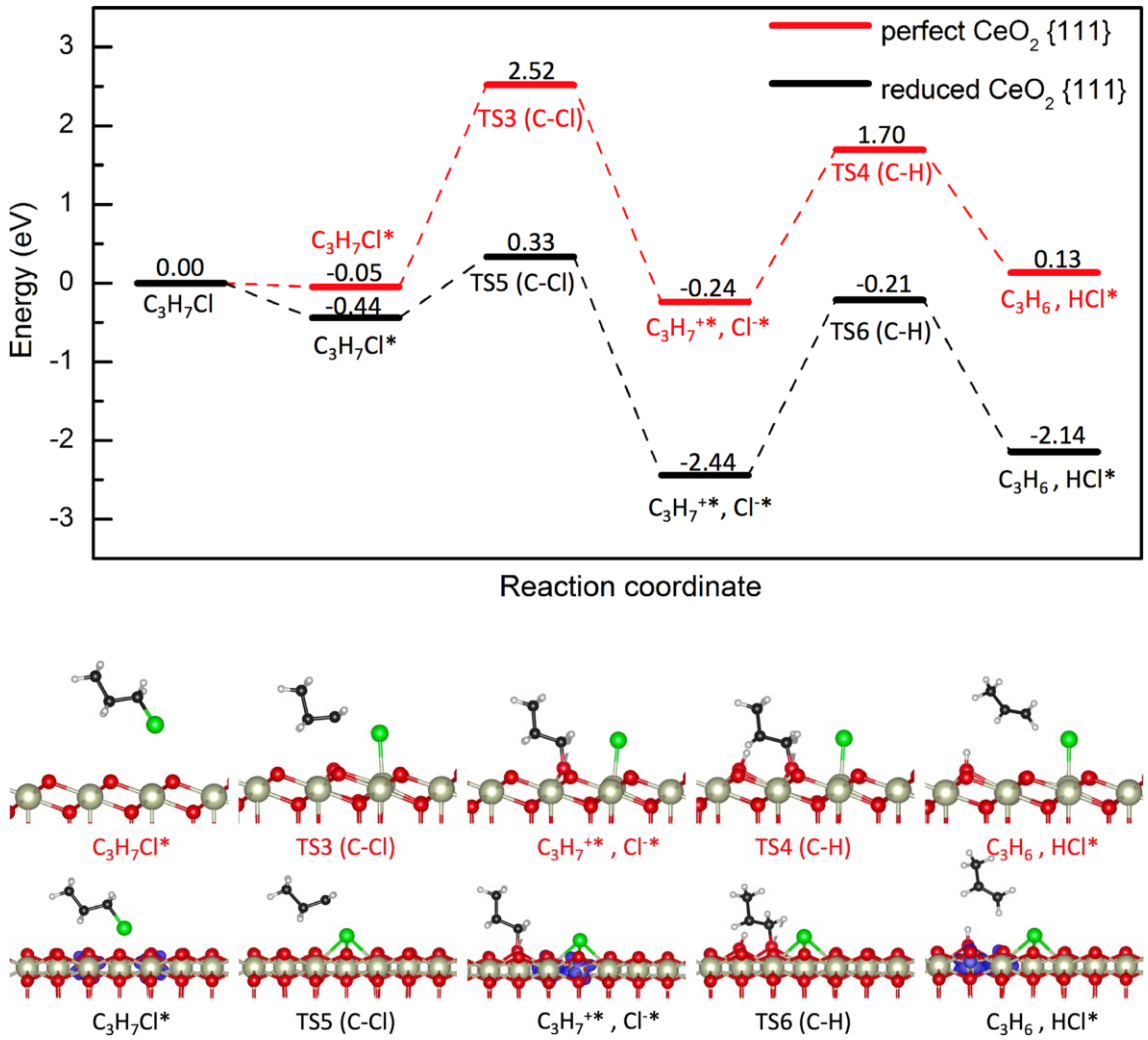

Figure S15. Calculated energy profiles and configurations for reaction pathway of C_3H_7Cl to C_3H_6.

3. Vibration frequencies for TS1-TS6 in Figure 12 and Figure S15

In order to prove the accuracy of the transition state on potential energy surfaces, we have calculated the vibration frequencies for each transition-state structure (TS), including TS1-TS6. All the calculated results are shown as follows. Vibrational frequencies have further been analyzed to confirm the transition state with only one imaginary (in red).

Vibration frequencies for TS1 in Figure 12

1	f =	91.771203 THz	576.615472 2PiTHz	3061.157726 cm-1	379.535323 meV
2	f =	91.297158 THz	573.636962 2PiTHz	3045.345297 cm-1	377.574831 meV
3	f =	91.087345 THz	572.318669 2PiTHz	3038.346693 cm-1	376.707114 meV
4	f =	89.776611 THz	564.083080 2PiTHz	2994.625295 cm-1	371.286350 meV
5	f =	89.546498 THz	562.637238 2PiTHz	2986.949554 cm-1	370.334679 meV
6	f =	88.992119 THz	559.153976 2PiTHz	2968.457484 cm-1	368.041954 meV
7	f =	88.470357 THz	555.875644 2PiTHz	2951.053352 cm-1	365.884116 meV
8	f =	45.949309 THz	288.708020 2PiTHz	1532.703906 cm-1	190.031133 meV
9	f =	44.051458 THz	276.783476 2PiTHz	1469.398441 cm-1	182.182253 meV
10	f =	43.422443 THz	272.831259 2PiTHz	1448.416763 cm-1	179.580856 meV
11	f =	43.159013 THz	271.176077 2PiTHz	1439.629674 cm-1	178.491395 meV
12	f =	42.109424 THz	264.581313 2PiTHz	1404.619142 cm-1	174.150641 meV
13	f =	40.444467 THz	254.120081 2PiTHz	1349.082165 cm-1	167.264931 meV
14	f =	38.819559 THz	243.910480 2PiTHz	1294.881051 cm-1	160.544847 meV
15	f =	38.355330 THz	240.993646 2PiTHz	1279.396058 cm-1	158.624952 meV
16	f =	37.529761 THz	235.806441 2PiTHz	1251.858027 cm-1	155.210670 meV
17	f =	34.716897 THz	218.132699 2PiTHz	1158.031007 cm-1	143.577598 meV
18	f =	34.438542 THz	216.383739 2PiTHz	1148.746065 cm-1	142.426411 meV
19	f =	31.993206 THz	201.019240 2PiTHz	1067.178436 cm-1	132.313310 meV
20	f =	30.741484 THz	193.154440 2PiTHz	1025.425497 cm-1	127.136604 meV
21	f =	27.048984 THz	169.953778 2PiTHz	902.256955 cm-1	111.865645 meV
22	f =	26.484668 THz	166.408074 2PiTHz	883.433388 cm-1	109.531820 meV
23	f =	26.127090 THz	164.161345 2PiTHz	871.505870 cm-1	108.052996 meV
24	f =	22.327593 THz	140.288402 2PiTHz	744.768303 cm-1	92.339534 meV
25	f =	13.360992 THz	83.949591 2PiTHz	445.674718 cm-1	55.256642 meV
26	f =	10.906958 THz	68.530435 2PiTHz	363.816931 cm-1	45.107567 meV
27	f =	8.920752 THz	56.050739 2PiTHz	297.564255 cm-1	36.893279 meV
28	f =	8.634319 THz	54.251024 2PiTHz	288.009858 cm-1	35.708684 meV
29	f =	7.062766 THz	44.376668 2PiTHz	235.588508 cm-1	29.209263 meV
30	f =	5.615705 THz	35.284515 2PiTHz	187.319752 cm-1	23.224698 meV
31	f =	4.494224 THz	28.238040 2PiTHz	149.911158 cm-1	18.586621 meV
32	f =	3.393903 THz	21.324524 2PiTHz	113.208430 cm-1	14.036061 meV
33	f =	2.858321 THz	17.959359 2PiTHz	95.343315 cm-1	11.821069 meV
34	f =	2.599453 THz	16.332848 2PiTHz	86.708430 cm-1	10.750479 meV
35	f =	1.989089 THz	12.497814 2PiTHz	66.348860 cm-1	8.226213 meV
36	f =	1.946023 THz	12.227225 2PiTHz	64.912348 cm-1	8.048108 meV
37	f=	1.540078 THz	9.676597 2PiTHz	51.371479 cm-1	6.369254 meV

38	f =	0.645930 THz	4.058496 2PiTHz	21.545893 cm-1	2.671351 meV
39	**f/i=**	**12.105988 THz**	**76.064164 2PiTHz**	**403.812272 cm-1**	**50.066359 meV**

Vibration frequencies for TS2 in Figure 12

1	f =	38.095377 THz	239.360311 2PiTHz	1270.724945 cm-1	157.549870 meV
2	f =	34.111172 THz	214.326815 2PiTHz	1137.826190 cm-1	141.072519 meV
3	f =	31.021929 THz	194.916532 2PiTHz	1034.780153 cm-1	128.296434 meV
4	f =	27.401591 THz	172.169274 2PiTHz	914.018662 cm-1	113.323912 meV
5	f =	17.345888 THz	108.987429 2PiTHz	578.596527 cm-1	71.736852 meV
6	f =	11.075223 THz	69.587676 2PiTHz	369.429650 cm-1	45.803455 meV
7	f =	7.243878 THz	45.514626 2PiTHz	241.629742 cm-1	29.958281 meV
8	f =	2.514760 THz	15.800705 2PiTHz	83.883372 cm-1	10.400216 meV
9	**f/i =**	**59.794563 THz**	**375.700321 2PiTHz**	**1994.531877 cm-1**	**247.290525 meV**

Vibration frequencies for TS3 in Figure S15

1	f =	96.611739 THz	607.029457 2PiTHz	3222.620624 cm-1	399.554178 meV
2	f =	93.270787 THz	586.037637 2PiTHz	3111.178465 cm-1	385.737106 meV
3	f =	92.286035 THz	579.850259 2PiTHz	3078.330682 cm-1	381.664499 meV
4	f =	91.688089 THz	576.093253 2PiTHz	3058.385350 cm-1	379.191592 meV
5	f =	91.538723 THz	575.154762 2PiTHz	3053.403054 cm-1	378.573866 meV
6	f =	90.368033 THz	567.799096 2PiTHz	3014.353020 cm-1	373.732277 meV
7	f =	89.219812 THz	560.584612 2PiTHz	2976.052498 cm-1	368.983616 meV
8	f =	44.004459 THz	276.488173 2PiTHz	1467.830726 cm-1	181.987881 meV
9	f =	43.292565 THz	272.015209 2PiTHz	1444.084488 cm-1	179.043722 meV
10	f =	42.724244 THz	268.444341 2PiTHz	1425.127328 cm-1	176.693333 meV
11	f =	42.532970 THz	267.242532 2PiTHz	1418.747120 cm-1	175.902288 meV
12	f =	39.996274 THz	251.303999 2PiTHz	1334.132042 cm-1	165.411351 meV
13	f =	37.001959 THz	232.490165 2PiTHz	1234.252461 cm-1	153.027857 meV
14	f =	36.678352 THz	230.456885 2PiTHz	1223.458108 cm-1	151.689527 meV
15	f =	35.143481 THz	220.813003 2PiTHz	1172.260307 cm-1	145.341807 meV
16	f =	34.289509 THz	215.447340 2PiTHz	1143.774874 cm-1	141.810062 meV
17	f =	28.063697 THz	176.329409 2PiTHz	936.104144 cm-1	116.062164 meV
18	f =	27.628528 THz	173.595161 2PiTHz	921.588468 cm-1	114.262448 meV
19	f =	26.275567 THz	165.094259 2PiTHz	876.458562 cm-1	108.667051 meV
20	f =	25.097115 THz	157.689826 2PiTHz	837.149628 cm-1	103.793363 meV
21	f =	23.899941 THz	150.167757 2PiTHz	797.216191 cm-1	98.842246 meV
22	f =	17.798639 THz	111.832145 2PiTHz	593.698664 cm-1	73.609279 meV
23	f =	13.193760 THz	82.898842 2PiTHz	440.096462 cm-1	54.565027 meV
24	f =	9.214071 THz	57.893715 2PiTHz	307.348313 cm-1	38.106348 meV
25	f =	8.037989 THz	50.504176 2PiTHz	268.118453 cm-1	33.242463 meV
26	f =	6.601579 THz	41.478942 2PiTHz	220.204954 cm-1	27.301945 meV
27	f =	5.956908 THz	37.428356 2PiTHz	198.701051 cm-1	24.635799 meV
28	f =	5.502707 THz	34.574526 2PiTHz	183.550532 cm-1	22.757374 meV
29	f =	5.274204 THz	33.138799 2PiTHz	175.928492 cm-1	21.812361 meV
30	f =	5.212214 THz	32.749304 2PiTHz	173.860728 cm-1	21.555991 meV
31	f =	4.529291 THz	28.458377 2PiTHz	151.080892 cm-1	18.731650 meV
32	f =	4.120885 THz	25.892284 2PiTHz	137.457924 cm-1	17.042617 meV
33	f =	3.554872 THz	22.335923 2PiTHz	118.577779 cm-1	14.701776 meV

34	f =	2.517811 THz	15.819874 2PiTHz	83.985139 cm-1	10.412834 meV
35	f =	2.247716 THz	14.122815 2PiTHz	74.975726 cm-1	9.295809 meV
36	f =	1.864375 THz	11.714216 2PiTHz	62.188868 cm-1	7.710440 meV
37	f =	1.574386 THz	9.892159 2PiTHz	52.515861 cm-1	6.511139 meV
38	f =	0.834375 THz	5.242530 2PiTHz	27.831738 cm-1	3.450697 meV
39	**f/i=**	**7.779275 THz**	**48.878626 2PiTHz**	**259.488675 cm-1**	**32.172507 meV**

Vibration frequencies for TS4 in Figure S15

1	f =	91.564986 THz	575.319774 2PiTHz	3054.279072 cm-1	378.682478 meV
2	f =	89.729264 THz	563.785594 2PiTHz	2993.045991 cm-1	371.090541 meV
3	f =	88.457009 THz	555.791780 2PiTHz	2950.608130 cm-1	365.828915 meV
4	f =	87.910777 THz	552.359701 2PiTHz	2932.387783 cm-1	363.569879 meV
5	f =	86.279812 THz	542.112046 2PiTHz	2877.984649 cm-1	356.824748 meV
6	f =	84.709943 THz	532.248270 2PiTHz	2825.619467 cm-1	350.332290 meV
7	f =	43.061346 THz	270.562418 2PiTHz	1436.371857 cm-1	178.087477 meV
8	f =	42.850237 THz	269.235982 2PiTHz	1429.330025 cm-1	177.214401 meV
9	f =	42.275945 THz	265.627597 2PiTHz	1410.173693 cm-1	174.839318 meV
10	f =	40.574384 THz	254.936371 2PiTHz	1353.415715 cm-1	167.802223 meV
11	f =	39.777997 THz	249.932528 2PiTHz	1326.851126 cm-1	164.508632 meV
12	f =	39.107642 THz	245.720559 2PiTHz	1304.490470 cm-1	161.736263 meV
13	f =	37.530429 THz	235.810642 2PiTHz	1251.880332 cm-1	155.213435 meV
14	f =	35.939106 THz	225.812063 2PiTHz	1198.799502 cm-1	148.632249 meV
15	f =	35.096197 THz	220.515912 2PiTHz	1170.683101 cm-1	145.146258 meV
16	f =	33.120073 THz	208.099557 2PiTHz	1104.766688 cm-1	136.973661 meV
17	f =	32.145393 THz	201.975461 2PiTHz	1072.254858 cm-1	132.942707 meV
18	f =	31.834439 THz	200.021677 2PiTHz	1061.882539 cm-1	131.656703 meV
19	f =	27.353462 THz	171.866870 2PiTHz	912.413250 cm-1	113.124866 meV
20	f =	26.695275 THz	167.731358 2PiTHz	890.458490 cm-1	110.402822 meV
21	f =	24.384568 THz	153.212759 2PiTHz	813.381610 cm-1	100.846503 meV
22	f =	22.835849 THz	143.481868 2PiTHz	761.721892 cm-1	94.441512 meV
23	f =	12.727816 THz	79.971227 2PiTHz	424.554231 cm-1	52.638035 meV
24	f =	9.504358 THz	59.717643 2PiTHz	317.031252 cm-1	39.306880 meV
25	f =	9.211192 THz	57.875627 2PiTHz	307.252286 cm-1	38.094442 meV
26	f =	8.262232 THz	51.913137 2PiTHz	275.598398 cm-1	34.169859 meV
27	f =	7.506403 THz	47.164120 2PiTHz	250.386641 cm-1	31.043998 meV
28	f =	6.683716 THz	41.995024 2PiTHz	222.944749 cm-1	27.641636 meV
29	f =	6.424659 THz	40.367321 2PiTHz	214.303537 cm-1	26.570262 meV
30	f =	5.080668 THz	31.922775 2PiTHz	169.472821 cm-1	21.011959 meV
31	f =	3.829112 THz	24.059022 2PiTHz	127.725432 cm-1	15.835941 meV
32	f =	2.882514 THz	18.111371 2PiTHz	96.150324 cm-1	11.921125 meV
33	f =	2.722297 THz	17.104698 2PiTHz	90.806060 cm-1	11.258521 meV
34	f =	2.041785 THz	12.828910 2PiTHz	68.106598 cm-1	8.444145 meV
35	f =	1.791845 THz	11.258493 2PiTHz	59.769507 cm-1	7.410477 meV
36	**f/i=**	**34.142191 THz**	**214.521711 2PiTHz**	**1138.860859 cm-1**	**141.200801 meV**

Vibration frequencies for TS5 in Figure S15

1	f =	95.860271 THz	602.307845 2PiTHz	3197.554349 cm-1	396.446355 meV
2	f =	92.766315 THz	582.867949 2PiTHz	3094.351108 cm-1	383.650779 meV
3	f =	91.916157 THz	577.526249 2PiTHz	3065.992890 cm-1	380.134807 meV
4	f =	91.548545 THz	575.216470 2PiTHz	3053.730652 cm-1	378.614483 meV
5	f =	90.595407 THz	569.227733 2PiTHz	3021.937420 cm-1	374.672623 meV
6	f =	89.354579 THz	561.431379 2PiTHz	2980.547846 cm-1	369.540968 meV
7	f =	89.198373 THz	560.449904 2PiTHz	2975.337353 cm-1	368.894949 meV
8	f =	43.581137 THz	273.828362 2PiTHz	1453.710220 cm-1	180.237161 meV
9	f =	43.208493 THz	271.486966 2PiTHz	1441.280128 cm-1	178.696026 meV
10	f =	43.016162 THz	270.278515 2PiTHz	1434.864662 cm-1	177.900609 meV
11	f =	42.310877 THz	265.847079 2PiTHz	1411.338886 cm-1	174.983783 meV
12	f =	40.301533 THz	253.222001 2PiTHz	1344.314402 cm-1	166.673803 meV
13	f =	38.277916 THz	240.507238 2PiTHz	1276.813796 cm-1	158.304792 meV
14	f =	37.794423 THz	237.469362 2PiTHz	1260.686204 cm-1	156.305225 meV
15	f =	34.630050 THz	217.587023 2PiTHz	1155.134105 cm-1	143.218427 meV
16	f =	33.023050 THz	207.489941 2PiTHz	1101.530336 cm-1	136.572405 meV
17	f =	29.461154 THz	185.109887 2PiTHz	982.718274 cm-1	121.841581 meV
18	f =	26.846246 THz	168.679937 2PiTHz	895.494342 cm-1	111.027188 meV
19	f =	26.327339 THz	165.419547 2PiTHz	878.185462 cm-1	108.881160 meV
20	f =	24.913184 THz	156.534152 2PiTHz	831.014347 cm-1	103.032685 meV
21	f =	22.113326 THz	138.942124 2PiTHz	737.621130 cm-1	91.453397 meV
22	f =	14.043431 THz	88.237479 2PiTHz	468.438421 cm-1	58.078983 meV
23	f =	11.050668 THz	69.433398 2PiTHz	368.610611 cm-1	45.701908 meV
24	f =	10.576402 THz	66.453494 2PiTHz	352.790787 cm-1	43.740499 meV
25	f =	10.361116 THz	65.100813 2PiTHz	345.609622 cm-1	42.850147 meV
26	f =	8.657665 THz	54.397712 2PiTHz	288.788600 cm-1	35.805236 meV
27	f =	7.193134 THz	45.195795 2PiTHz	239.937121 cm-1	29.748422 meV
28	f =	4.515098 THz	28.369199 2PiTHz	150.607460 cm-1	18.672952 meV
29	f =	3.822823 THz	24.019503 2PiTHz	127.515633 cm-1	15.809929 meV
30	f =	3.147842 THz	19.778473 2PiTHz	105.000694 cm-1	13.018432 meV
31	f =	2.833450 THz	17.803090 2PiTHz	94.513711 cm-1	11.718211 meV
32	f =	2.164081 THz	13.597320 2PiTHz	72.185959 cm-1	8.949922 meV
33	f =	1.771021 THz	11.127652 2PiTHz	59.074896 cm-1	7.324356 meV
34	f =	1.272773 THz	7.997069 2PiTHz	42.455138 cm-1	5.263768 meV
35	f =	0.779553 THz	4.898079 2PiTHz	26.003103 cm-1	3.223975 meV
36	**f/i=**	**4.412732 THz**	**27.726013 2PiTHz**	**147.192891 cm-1**	**18.249599 meV**

Vibration frequencies for TS6 in Figure S15

1	f =	91.169604 THz	572.835515 2PiTHz	3041.090548 cm-1	377.047309 meV
2	f =	89.703578 THz	563.624204 2PiTHz	2992.189198 cm-1	370.984312 meV
3	f =	87.920601 THz	552.421428 2PiTHz	2932.715478 cm-1	363.610508 meV
4	f =	86.775949 THz	545.229367 2PiTHz	2894.534000 cm-1	358.876607 meV
5	f =	86.530103 THz	543.684669 2PiTHz	2886.333448 cm-1	357.859867 meV
6	f =	84.389020 THz	530.231852 2PiTHz	2814.914632 cm-1	349.005060 meV
7	f =	43.398489 THz	272.680751 2PiTHz	1447.617738 cm-1	179.481789 meV
8	f =	43.105840 THz	270.841984 2PiTHz	1437.856024 cm-1	178.271491 meV
9	f =	42.823211 THz	269.066170 2PiTHz	1428.428521 cm-1	177.102629 meV
10	f =	41.340812 THz	259.751981 2PiTHz	1378.981006 cm-1	170.971916 meV
11	f =	40.448042 THz	254.142541 2PiTHz	1349.201402 cm-1	167.279714 meV

12	f =	39.224672 THz	246.455881 2PiTHz	1308.394174 cm-1	162.220261 meV
13	f =	38.021873 THz	238.898474 2PiTHz	1268.273127 cm-1	157.245883 meV
14	f =	36.812279 THz	231.298373 2PiTHz	1227.925430 cm-1	152.243405 meV
15	f =	35.635449 THz	223.904129 2PiTHz	1188.670591 cm-1	147.376423 meV
16	f =	33.079091 THz	207.842056 2PiTHz	1103.399661 cm-1	136.804172 meV
17	f =	31.794530 THz	199.770923 2PiTHz	1060.551328 cm-1	131.491653 meV
18	f =	31.434072 THz	197.506097 2PiTHz	1048.527733 cm-1	130.000917 meV
19	f =	27.179082 THz	170.771211 2PiTHz	906.596574 cm-1	112.403690 meV
20	f =	26.316031 THz	165.348502 2PiTHz	877.808295 cm-1	108.834397 meV
21	f =	25.041852 THz	157.342594 2PiTHz	835.306231 cm-1	103.564811 meV
22	f =	23.213595 THz	145.855322 2PiTHz	774.322172 cm-1	96.003748 meV
23	f =	12.191297 THz	76.600181 2PiTHz	406.657896 cm-1	50.419171 meV
24	f =	9.924795 THz	62.359328 2PiTHz	331.055524 cm-1	41.045668 meV
25	f =	9.292952 THz	58.389340 2PiTHz	309.979506 cm-1	38.432574 meV
26	f =	8.627152 THz	54.205995 2PiTHz	287.770808 cm-1	35.679046 meV
27	f =	7.256981 THz	45.596953 2PiTHz	242.066807 cm-1	30.012470 meV
28	f =	5.947132 THz	37.366930 2PiTHz	198.374951 cm-1	24.595368 meV
29	f =	5.128106 THz	32.220840 2PiTHz	171.055196 cm-1	21.208149 meV
30	f =	4.632426 THz	29.106390 2PiTHz	154.521089 cm-1	19.158180 meV
31	f =	4.139387 THz	26.008538 2PiTHz	138.075096 cm-1	17.119136 meV
32	f =	3.814267 THz	23.965745 2PiTHz	127.230243 cm-1	15.774545 meV
33	f =	3.424296 THz	21.515485 2PiTHz	114.222211 cm-1	14.161754 meV
34	f =	2.374881 THz	14.921815 2PiTHz	79.217487 cm-1	9.821720 meV
35	f =	1.101497 THz	6.920911 2PiTHz	36.741991 cm-1	4.555428 meV
36	**f/i=**	**41.113599 THz**	**258.324363 2PiTHz**	**1371.402012 cm-1**	**170.032240 meV**

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