Supporting Information

Catalytic conversion of free fatty acids to bio-based aromatics: A model investigation using oleic acid and an H-ZSM-5/Al_2O_3 catalyst

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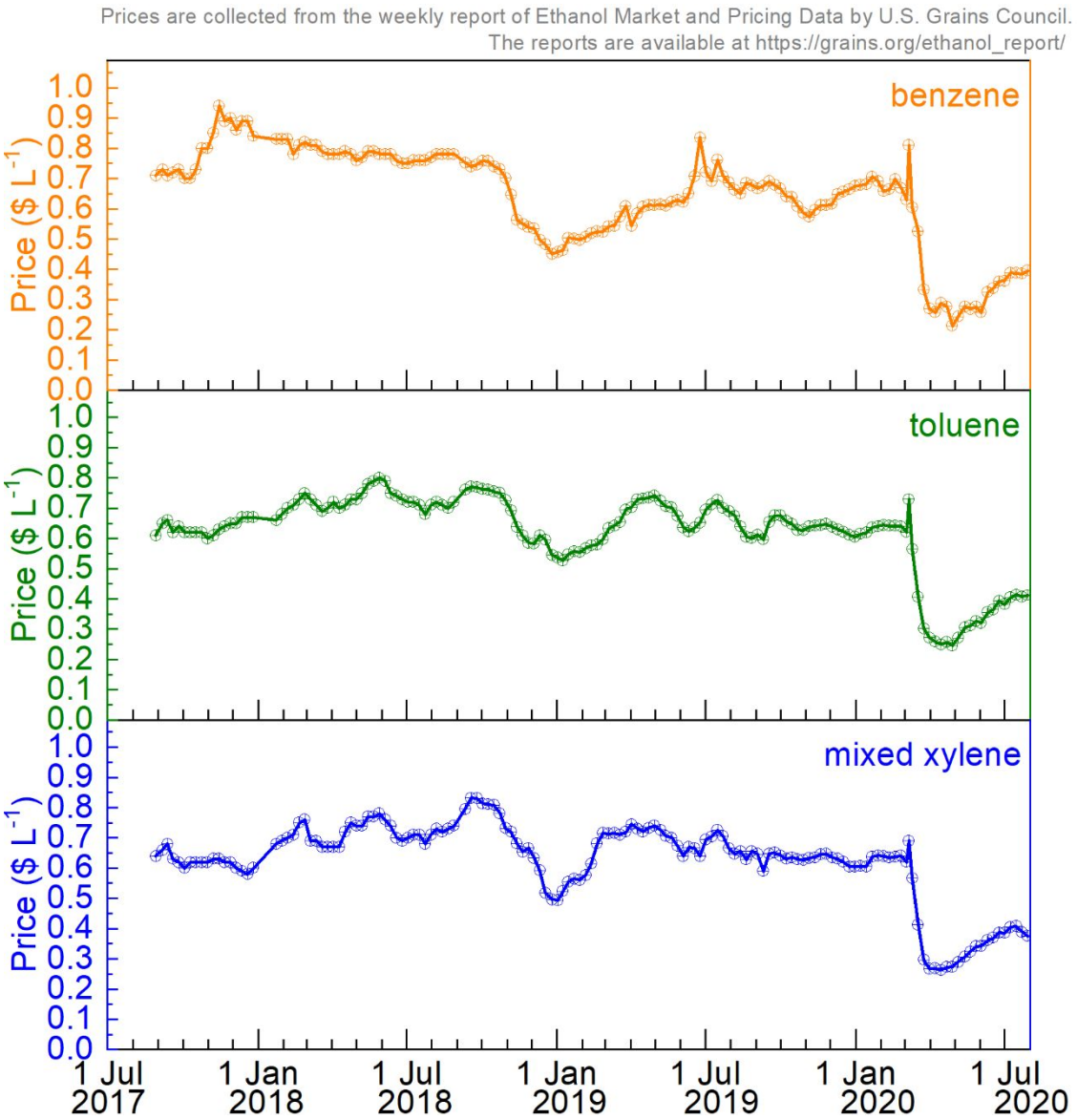


Fig. S1. Pricing for benzene, toluene, and mixed xylene in the past three years (1 July 2017 - 31 July 2020).

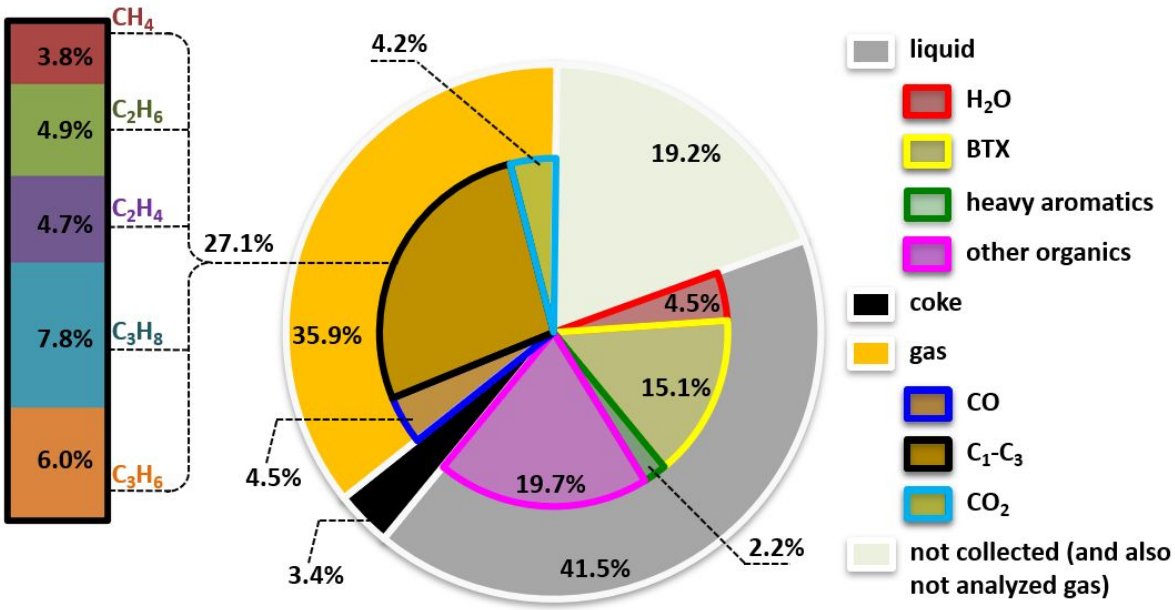


Fig. S2. Mass balance for catalytic conversion of oleic acid over fresh H-ZSM-5/Al_2O_3 catalyst. (Reaction conditions: catalyst particle size of 1.2 - 1.8 mm, catalyst loading of 10 g, catalyst bed temperature of 550 °C, atmospheric pressure, N_2 flow of 50 ml min^{-1}, and WHSV of oleic acid of 1 h^{-1}.)

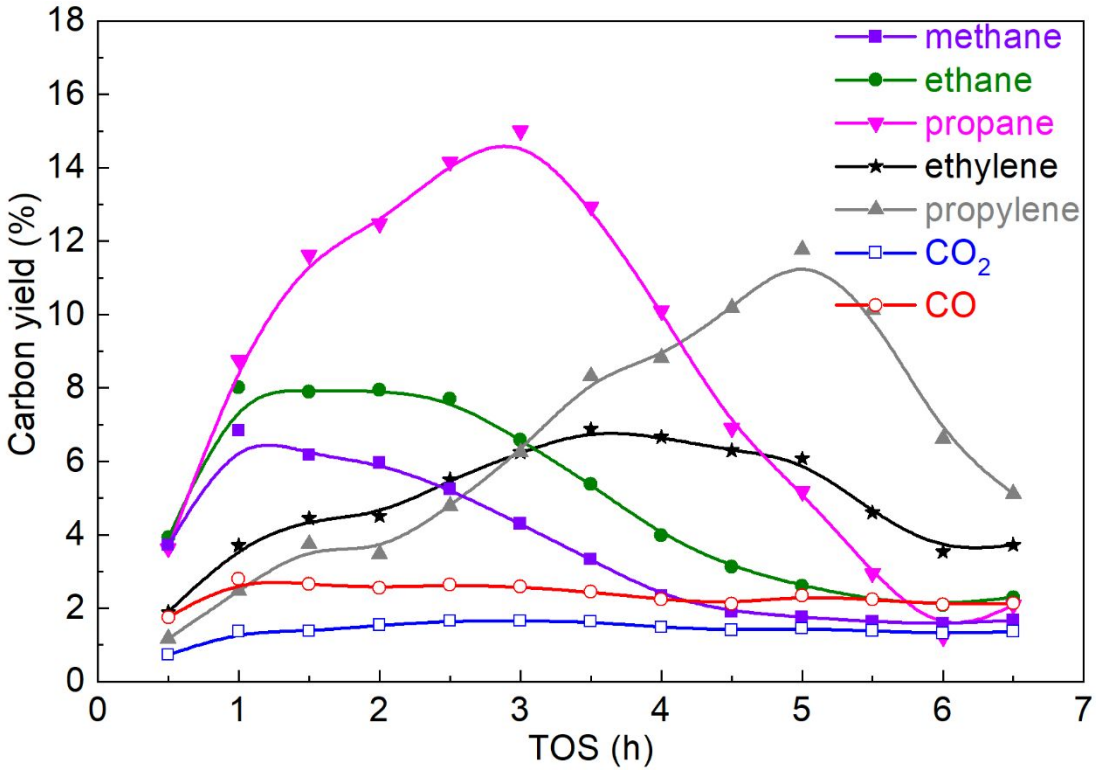


Fig. S3. Carbon yields of gaseous products *versus* TOS over fresh H-ZSM-5/Al_2O_3 catalysts. (Reaction conditions: catalyst particle size of 1.2 - 1.8 mm, catalyst loading of 10 g, catalyst bed temperature of 550 °C, atmospheric pressure, N_2 flow of 50 ml min^{-1}, and WHSV of oleic acid of 1 h^{-1}.)

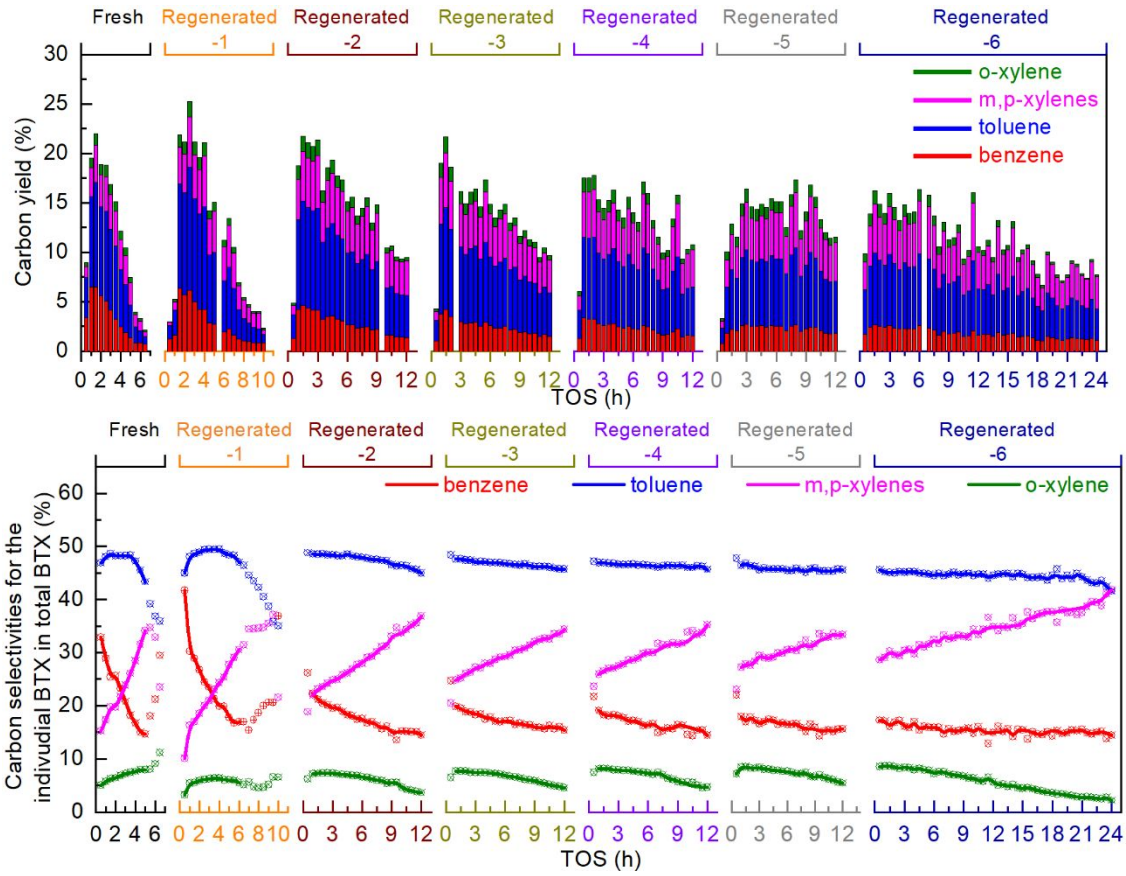


Fig. S4. Carbon yields of aromatics (top) and selectivity's of the individual BTX (bottom) *versus* TOS over fresh and regenerated H-ZSM-5/Al_2O_3 catalysts.

(Reaction conditions: catalyst particle size of 1.2 - 1.8 mm, catalyst loading of 10 g, catalyst bed temperature of 550 °C, atmospheric pressure, N_2 flow of 50 ml min^{-1}, and oleic acid feeding of 10 g h^{-1}.)

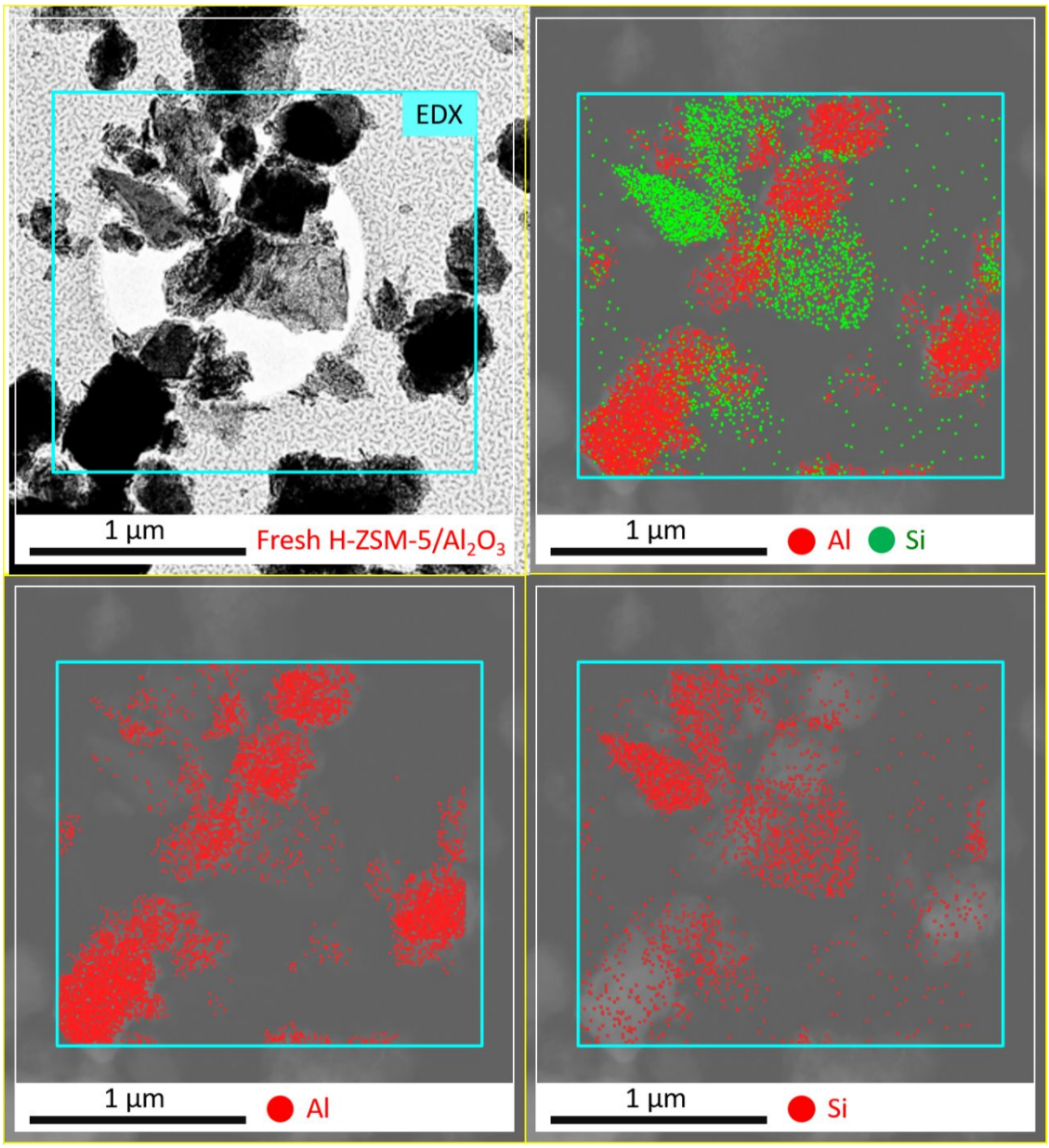
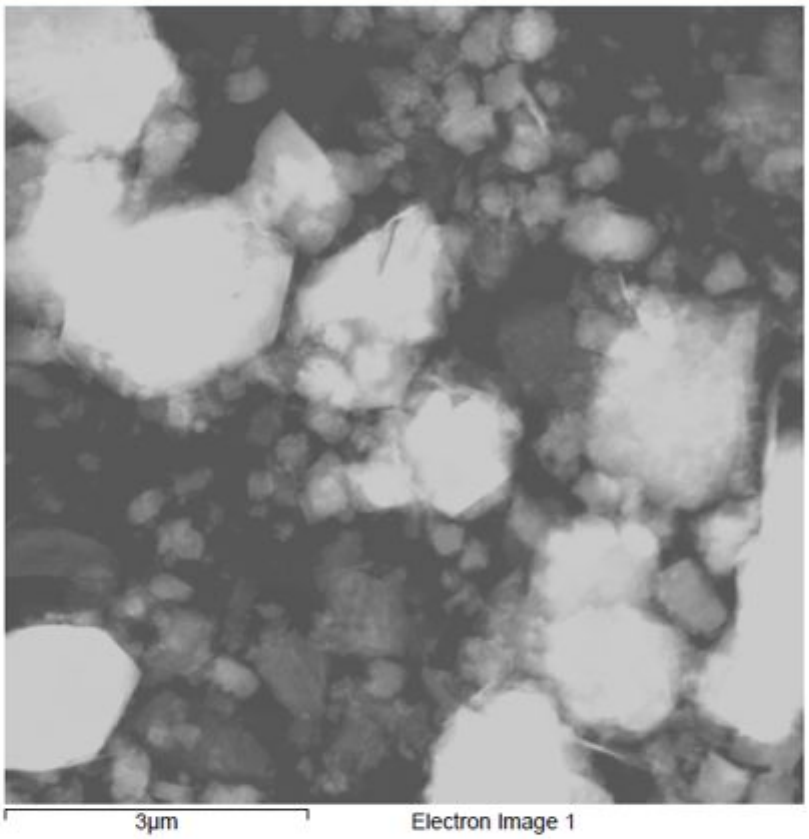


Fig. S5. TEM image and elemental (Al and Si) maps of the fresh H-ZSM-5/Al_2O_3 catalyst.



Spectrum processing :
Peak possibly omitted : 3.690 keV

Quantitation method : Cliff Lorimer thin ratio section.
Processing option : All elements analyzed
Number of iterations = 1

Standardless

Element	Weight%	Atomic%
C K	2.54	4.76
O K	39.20	55.18
Al K	20.04	16.72
Si K	21.89	17.55
Cu K	16.34	5.79
Totals	100.00	

Fig. S6. Quantitative EDX analysis of Fresh catalyst.

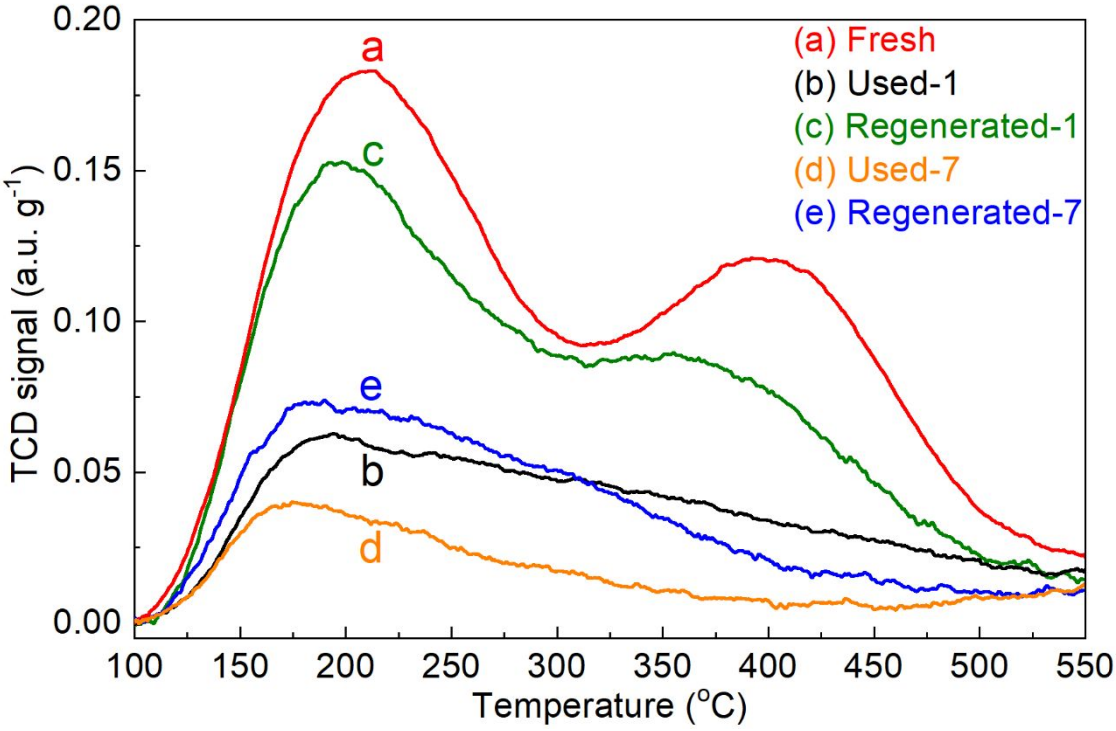


Fig. S7. NH_3-TPD profiles of fresh, used and regenerated H-ZSM-5/Al_2O_3 catalysts.

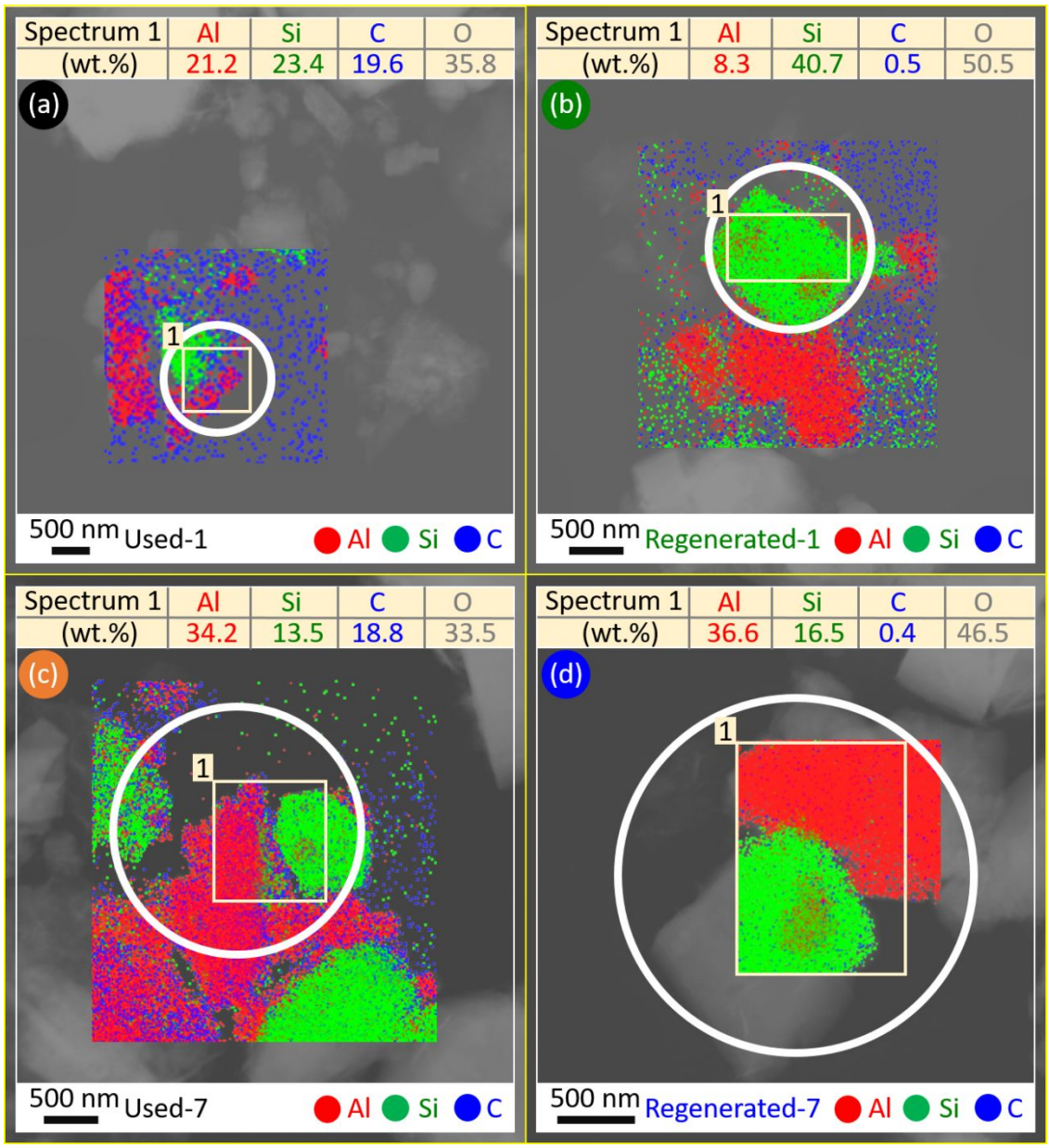


Fig. S8. Elemental (Al, Si and C) maps of the used and regenerated H-ZSM-5/Al_2O_3 catalysts. (The white circle means the hole on a carbon-coated copper grid used for TEM and EDX analyses.)

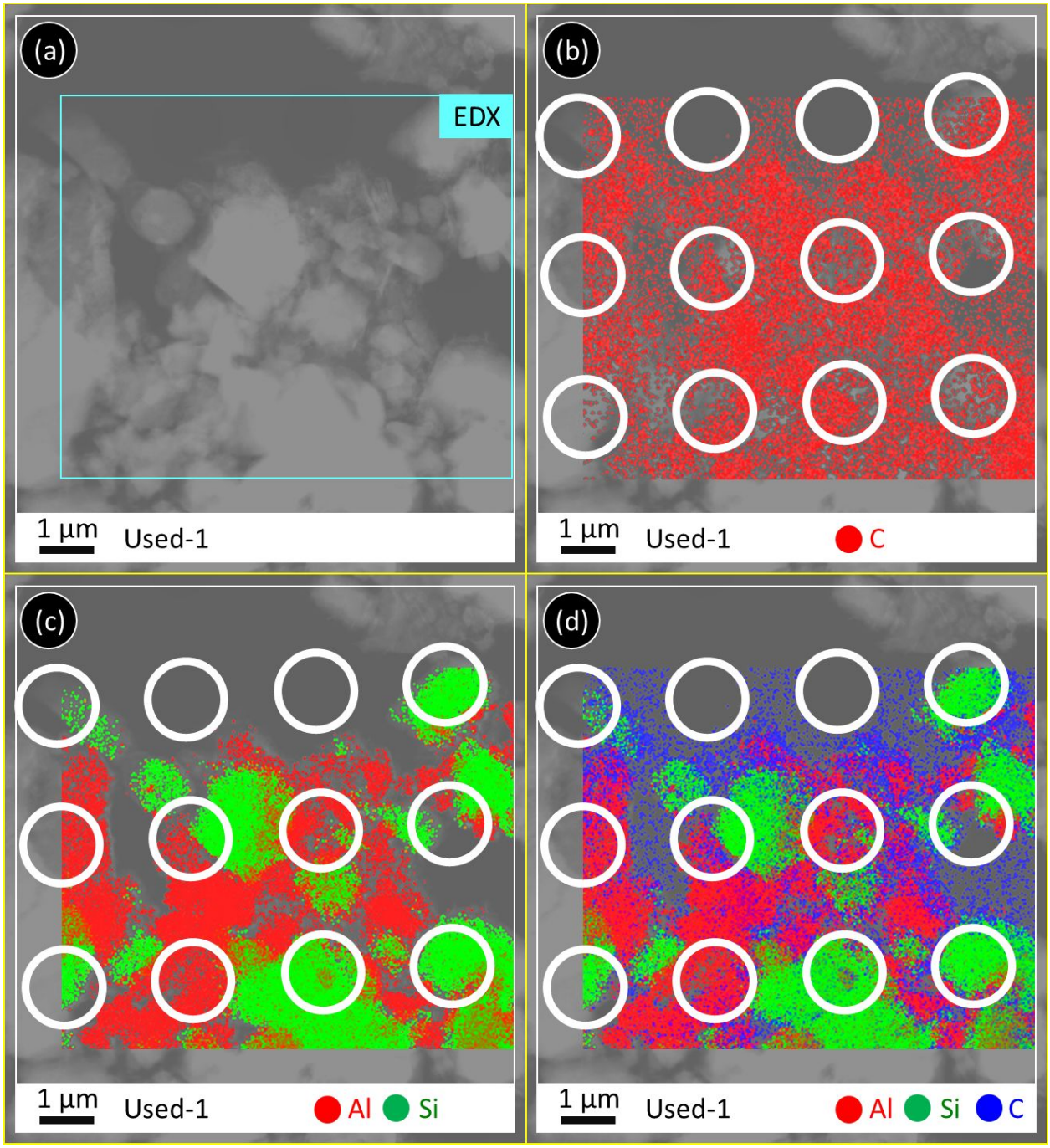


Fig. S9. Elemental (Al, Si and C) maps of Used-1 catalyst.

(The white circle means the holes on a carbon-coated copper grid used for TEM and EDX analyses.)

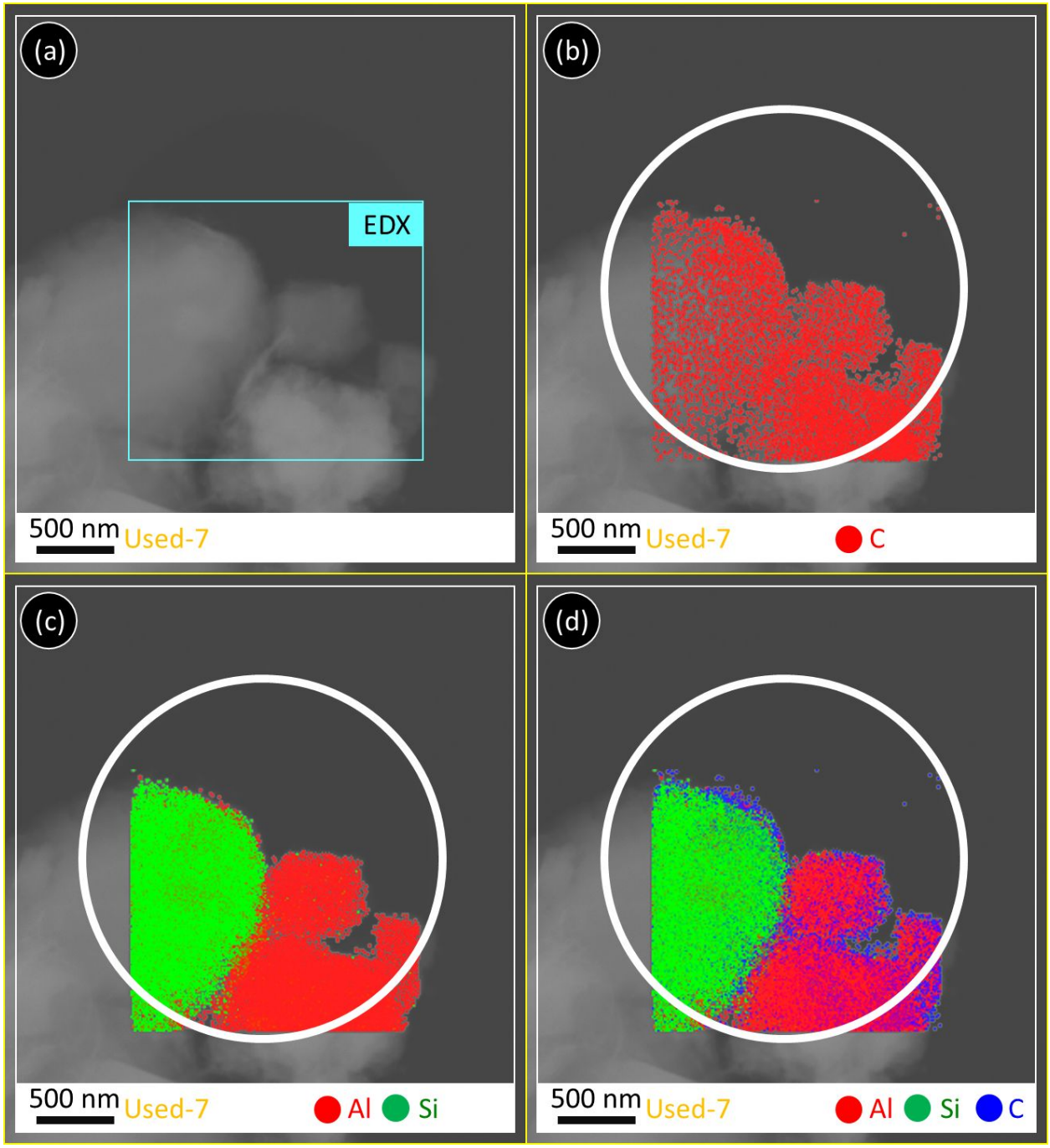
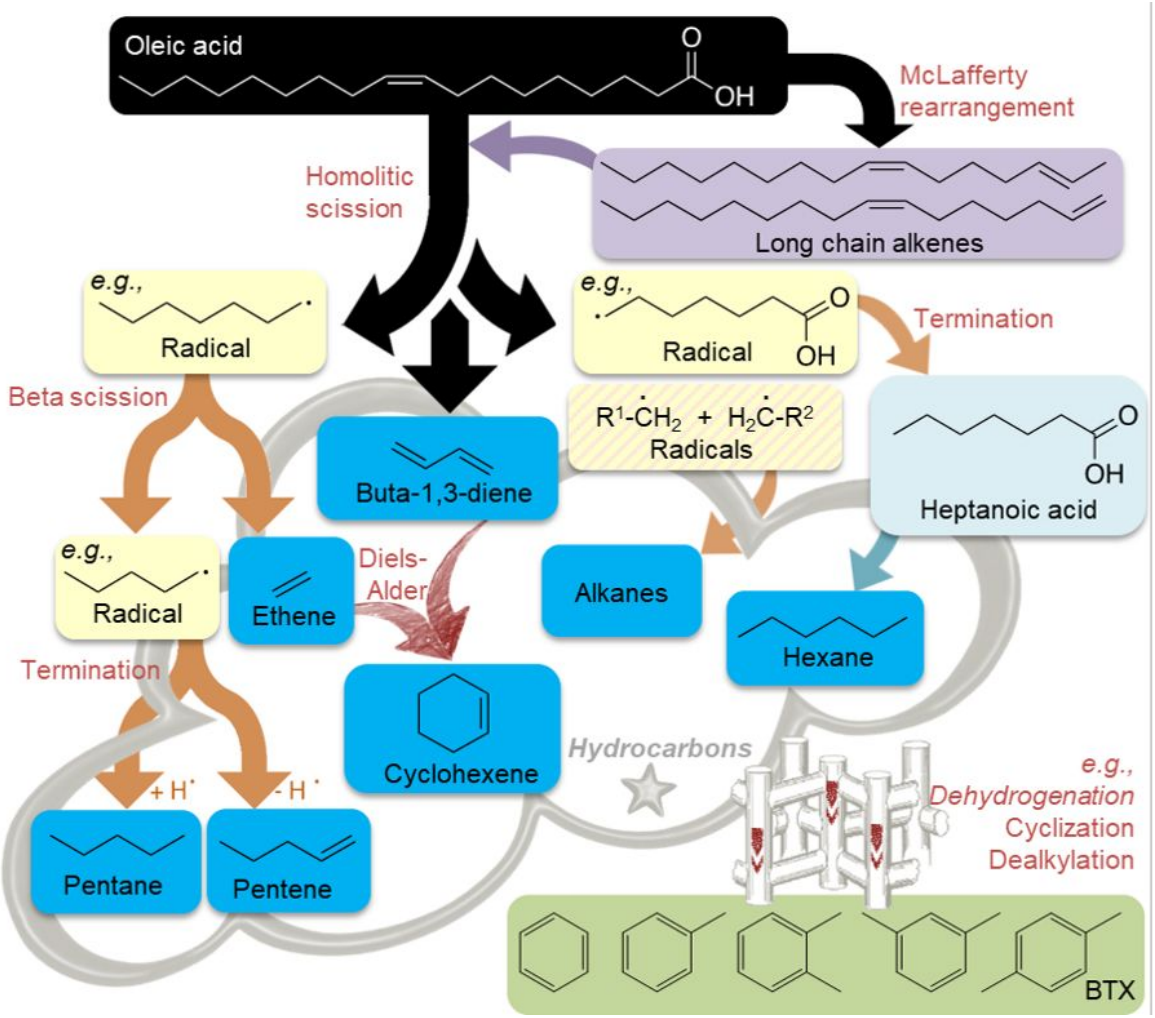


Fig. S10. Elemental (Al, Si and C) maps of Used-7 catalyst.

(The white circle means the hole on a carbon-coated copper grid used for TEM and EDX analyses.)



Scheme S1. Proposed reaction pathways for conversion of oleic acid to aromatics. [1-5]

Table S1 GC-MS analysis of the liquid product from thermal pyrolysis of oleic acid

R.T.	Library/ID	Quality	Area%
1.488	Propene	91	0.9
1.5405	Bicyclo[1.1.0]butane	87	2.1
1.6544	1-Pentene	90	2.5
1.7377	1,3-Pentadiene, (Z)-	98	0.6
1.7727	1,3-Cyclopentadiene	91	0.7
1.8297	Cyclopentene	91	1.5
1.9567	1-Hexene	95	3.7
2.0794	Cyclopentene, 4-methyl-	93	0.4
2.3554	Isopropenylcyclopropane	90	0.9
2.4387	Benzene	94	0.8
2.5087	Cyclopentene,3-methylene-	81	0.6
2.6051	Cyclohexene	94	1.3
2.684	1-Heptene	95	2.5
2.776	Heptane	95	0.9
3.0739	1,1'-Bicyclopropyl	53	0.7
3.1177	Vinylcyclopentane	94	0.5
3.3368	2-Heptyne	91	0.8
3.5514	Cyclopentane, ethylidene-	90	0.5
3.6785	1,3,5-Hexatriene, 3-methyl-, (Z)-	91	0.3
3.753	1,3,5-Cycloheptatriene	70	0.9
3.8143	Cyclohexene, 3-methyl-	94	0.6
4.0071	1,7-Octadiene	90	1.6
4.1735	1-Octene	95	2.1
4.3488	Octane	91	0.7
6.5525	1-Nonene	95	2.0
6.8197	Cyclooctene, (Z)-	91	3.4
8.1034	Cyclopentene, 1-butyl-	95	0.4
9.444	1-Decene	87	1.2
11.6389	Cyclodecene	90	0.3
12.4801	1-Nonene	97	1.4
12.8787	5-Undecene	94	0.8
13.1241	2-Undecene, (E)-	97	0.4
13.4921	1,7-Octadiene	80	0.8
15.4329	1-Dodecene	98	0.8
16.4011	1,2-Nonadiene	78	0.6
18.2499	1-Tridecene	98	0.6
20.918	Cyclooctane, methyl-	83	4.5
21.1195	n-Decanoic acid	98	3.5
22.4995	Cyclopentene, 1-pentyl-	72	0.7
22.8194	Cyclohexene, 1-octyl-	93	0.5
23.4415	1-Hexadecene	91	0.8
23.6474	Pentadecane	97	1.9

25.3297	Benzocyclodecene, tetradecahydro-	93	1.3
25.4217	Spiro[4.5]decane	94	0.8
25.7153	Dichloroacetic acid, 4-hexadecyl ester	94	0.5
26.758	Cyclopentane, 1,1,3-trimethyl-	64	0.5
26.8412	Spiro[4.5]decane	93	2.8
26.9639	8-Heptadecene	99	7.5
27.0208	8-Heptadecene	99	4.6
27.1084	E-14-Hexadecenal	99	0.8
27.1873	Heptadecane	95	1.4
27.7656	Z,Z-10,12-Hexadecadienal	92	0.3
27.9759	E-7-Octadecene	97	0.6
28.7031	1-Nonadecene	95	0.2
29.3822	n-Hexadecanoic acid	98	3.7
29.9868	Z,E-2,13-Octadecadien-1-ol	98	0.7
30.4599	Oleic acid	91	17.5
30.8981	11-Dodecen-1-ol difluoroacetate	91	1.0
31.8575	Z-11,13-Dimethyl-11-tetradecen-1-ol acetate	92	0.5
32.4095	Spiro[4.5]decane	91	2.8

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