

Supporting Information

for the manuscript

Topology of silica supported vanadium-titanium oxide catalysts for oxidative dehydrogenation of propane

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Table S1: Summary of chemical analysis and microstructural details for prepared catalysts

ID	Sample	V [wt%]	V [mmol/g _{cat}]	Ti [wt %]	Ti [mmol/g _{cat}]	Total [wt%]	Total [mmol/g _{cat}]	SBA-15 / Ti/SBA-15 mother	Pore diameter [nm]	S(BET) [m ² /g]	Micropore area [m ² /g]	SAXRD a ₀ [nm]	Wall thickness [nm]	Metal oxide layer thickness [nm]
7495	SBA-15	0.00	0.00	0.00	0.00	0.00	0.00	X	7.31	978.0	427.0	11.22	3.91	0.00
7569	3Ti/SBA-15	0.00	0.00	3.36	0.70	3.36	0.70	7495	7.03	823.0	316.0	10.97	3.94	0.01
7622	8Ti/SBA-15	0.00	0.00	8.31	1.74	8.31	1.74	7495	6.79	806.0	292.0	10.96	4.17	0.13
7606	1V/3Ti/SBA-15	0.98	0.19	3.29	0.69	4.27	0.88	7495/ 7569	7.03	757.0	293.0	10.96	3.93	0.01
7620	4V/3Ti/SBA-15	3.75	0.74	3.11	0.65	6.86	1.39	7495/ 7569	7.03	623.0	192.0	10.94	3.91	0.00
7624	4V/8Ti/SBA-15	3.81	0.75	7.61	1.59	11.42	2.34	7495/ 7622	6.79	317.0	79.0	10.84	4.05	0.07
7514	SBA-15	0.00	0.00	0.00	0.00	0.00	0.00	X	7.31	886.0	350.0	10.80	3.49	0.00
7724	SBA-15	0.00	0.00	0.00	0.00	0.00	0.00	X	7.31	987.0	381.0	10.90	3.59	0.00
7751	SBA-15	0.00	0.00	0.00	0.00	0.00	0.00	X	7.31	701.0	210.0	11.00	3.69	0.00
7671	1Ti/SBA-15	0.00	0.00	0.90	0.19	0.90	0.19	7514	6.79	841.0	332.0	10.83	4.04	0.27
7674	2Ti/SBA-15	0.00	0.00	1.82	0.38	1.82	0.38	7514	7.03	750.0	303.0	10.82	3.79	0.15
7676	3Ti/SBA-15	0.00	0.00	3.35	0.70	3.35	0.70	7514	7.03	815.0	317.0	10.84	3.81	0.16
7688	7Ti/SBA-15	0.00	0.00	6.81	1.42	6.81	1.42	7514	7.03	652.0	212.0	10.84	3.81	0.16
7731	9Ti/SBA-15	0.00	0.00	9.20	1.92	9.20	1.92	7724	6.79	755.0	263.0	10.91	4.12	0.26
7734	14Ti/SBA-15	0.00	0.00	14.08	2.94	14.08	2.94	7724	2 peaks	651.0	186.0	10.86	n/a	n/a
7779	1V/SBA-15	0.99	0.20	0.00	0.00	0.99	0.20	7724	7.03	939.0	345.0	10.97	3.94	0.17
7802	2V/SBA-15	1.77	0.35	0.00	0.00	1.77	0.35	7724	7.03	926.0	335.0	10.92	3.89	0.15
7815	3.5V/SBA-15	3.45	0.68	0.00	0.00	3.45	0.68	7751	7.31	807.0	212.0	10.89	3.58	0.00
7817	6.5V/SBA-15	6.34	1.24	0.00	0.00	6.34	1.24	7751	7.31	679.0	129.0	10.89	3.58	0.00
7827	9V/SBA-15	9.15	1.80	0.00	0.00	9.15	1.80	7751	7.03	529.0	80.0	10.89	3.85	0.08
9093	SBA-15	0.00	0.00	0.00	0.00	0.00	0.00	X	7.31	821.2	257.5	10.84	3.53	0.00
9181	4V/SBA-15	3.56	0.70	0.00	0.00	3.56	0.70	9093	7.31	773.5	191.0	10.91	3.60	0.04
9183	4V/SBA-15	3.91	0.77	0.00	0.00	3.91	0.77	9093	7.31	748.6	182.1	10.94	3.63	0.01
9575	1Ti/SBA-15	0.00	0.00	0.92	0.19	0.92	0.19	9093	7.31	921.2	293.9	10.90	3.59	0.03
10429	4V/1Ti/SBA-15	4.18	0.82	1.17	0.24	5.35	1.06	9093/ 9575	7.31	680.4	163.6	10.90	3.59	0.00
8759	SBA-15	0.00	0.00	0.00	0.00	0.00	0.00	X	6.79	812.3	347.8	10.60	3.81	0.00
9576	2Ti/SBA-15	0.00	0.00	1.74	0.36	1.74	0.36	8759	6.79	752.2	315.5	10.59	3.80	0.00
10190	1V/2Ti/SBA-15	0.80	0.16	1.75	0.37	2.55	0.52	8759/ 9576	6.79	704.1	280.7	10.63	3.84	0.02

10205	3V/2Ti/SBA-15	2.76	0.54	1.67	0.35	4.43	0.89	8759/ 9576	6.79	664.7	245.6	10.56	3.77	0.00
10207	4V/2Ti/SBA-15	3.44	0.68	1.69	0.35	5.13	1.03	8759/ 9576	6.79	600.7	195.8	10.56	3.77	0.00
10209	6V/2Ti/SBA-15	5.66	1.11	1.60	0.33	7.26	1.45	8759/ 9576	6.79	542.6	160.1	10.53	3.74	0.00
8814	SBA-15	0.00	0.00	0.00	0.00	0.00	0.00	X	7.31	881.8	332.0	10.93	3.62	0.00
8871	3Ti/SBA-15	0.00	0.00	3.17	0.66	3.17	0.66	8814	7.03	814.0	305.6	10.88	3.85	0.11
9018	1V/3Ti/SBA-15	1.27	0.25	3.04	0.64	4.31	0.88	8814/ 8871	7.03	725.6	251.8	10.88	3.85	0.11
9019	2V/3Ti/SBA-15	2.19	0.43	3.03	0.63	5.22	1.06	8814/ 8871	7.03	707.6	240.7	10.87	3.84	0.11
9020	3V/3Ti/SBA-15	3.21	0.63	2.99	0.62	6.20	1.25	8814/ 8871	7.03	656.8	202.9	10.85	3.82	0.10
9021	6V/3Ti/SBA-15	6.09	1.20	2.79	0.58	8.88	1.78	8814/ 8871	7.03	498.1	113.1	10.74	3.71	0.04
8886	SBA-15	0.00	0.00	0.00	0.00	0.00	0.00	X	7.03	849.1	305.2	10.47	3.44	0.00
9238	11Ti/SBA-15	0.00	0.00	10.97	2.29	10.97	2.29	8886	6.56	596.1	177.7	10.44	3.88	0.22
9240	14Ti/SBA-15	0.00	0.00	13.97	2.92	13.97	2.92	8886	6.56	527.6	148.4	10.33	3.77	0.17
9507	4V/13Ti/SBA-15	4.35	0.85	12.70	2.65	17.05	3.51	8886/ 9240	6.32	395.4	46.2	10.32	4.00	0.28
9514	17Ti/SBA-15	0.00	0.00	16.71	3.49	16.71	3.49	8886	6.56	439.4	104.0	10.29	3.73	0.15
12478	2V/17Ti/SBA-15	1.81	0.36	16.89	3.53	18.70	3.88	9514	6.08	372.5	98.2	10.15	4.07	0.09
12479	4V/17Ti/SBA-15	3.87	0.76	16.25	3.40	20.12	4.15	9514	5.88	345.1	62.3	10.14	4.26	0.19
12480	6V/17Ti/SBA-15	6.46	1.27	14.71	3.07	21.17	4.34	9514	6.32	330.6	96.3	10.22	3.90	0.01
9179	SBA-15	0.00	0.00	0.00	0.00	0.00	0.00	X	6.56	757.9	307.7	10.30	3.74	0.00
9809	7Ti/SBA-15	0.00	0.00	6.68	1.40	6.68	1.40	9179	6.56	648.2	233.6	10.23	3.67	0.00
9811	11Ti/SBA-15	0.00	0.00	11.00	2.30	11.00	2.30	9179	6.32	574.3	183.4	10.20	3.88	0.10
10283	17Ti/SBA-15	0.00	0.00	17.51	3.66	17.51	3.66	9179	5.88	442.7	66.7	10.20	4.32	0.29
10312	19Ti/SBA-15	0.00	0.00	19.35	4.04	19.35	4.04	9179	5.88	404.0	19.2	10.17	4.29	0.27
10314	21Ti/SBA-15	0.00	0.00	20.99	4.39	20.99	4.39	9179	5.88	372.5	0.4	10.14	4.26	0.29
9846	14Ti/SBA-15	0.00	0.00	14.48	3.03	14.48	3.03	9179	6.08	503.9	143.5	10.23	4.15	0.23
10179	1V/14Ti/SBA-15	0.56	0.11	14.04	2.93	14.60	3.04	9179/ 9846	6.08	493.7	129.4	10.21	4.13	0.22
10180	2V/14Ti/SBA-15	1.48	0.29	13.74	2.87	15.22	3.16	9179/ 9846	6.08	466.3	106.9	10.21	4.13	0.22
10181	3V/14Ti/SBA-15	2.92	0.57	13.43	2.81	16.35	3.38	9179/ 9846	6.08	435.4	84.9	10.23	4.15	0.23
9954	4V/14Ti/SBA-15	4.04	0.79	13.19	2.76	17.23	3.55	9179/ 9846	5.88	427.7	76.1	10.23	4.35	0.23
10182	6V/14Ti/SBA-15	5.71	1.12	12.62	2.64	18.33	3.76	9179/ 9846	5.88	349.7	0.0	10.19	4.31	0.31
10380	23Ti/SBA-15	0.00	0.00	22.62	4.73	22.62	4.73	9179	5.68	358.4	0.0	10.05	4.37	0.34
10413	1V/23Ti/SBA-15	0.86	0.17	22.11	4.62	22.97	4.79	9179/ 10380	5.48	305.9	21.7	10.03	4.55	0.40
10415	2V/23Ti/SBA-15	2.00	0.39	21.57	4.51	23.57	4.90	9179/ 10380	5.48	293.0	17.2	10.02	4.54	0.43
10417	3V/23Ti/SBA-15	3.21	0.63	21.08	4.40	24.29	5.03	9179/ 10380	5.29	300.9	8.5	10.06	4.78	0.45

10419	4V/23Ti/SBA-15	4.51	0.89	20.50	4.28	25.01	5.17	9179/ 10380	5.29	270.7	0.0	10.03	4.75	0.21
10421	7V/23Ti/SBA-15	6.58	1.29	19.76	4.13	26.34	5.42	9179/ 10380	5.29	221.7	0.0	error	n/a	n/a
11780	SBA-15	0.00	0.00	0.00	0.00	0.00	0.00	X	7.06	817.7	314.4	10.97	3.91	0.00
11807	7Ti/SBA-15	0.00	0.00	6.96	1.45	6.96	1.45	11780	7.04	580.8	177.0	10.73	3.69	0.00
11815	12Ti/SBA-15	0.00	0.00	11.56	2.42	11.56	2.42	11780	6.72	441.2	82.3	10.57	3.85	0.00
11817	15Ti/SBA-15	0.00	0.00	14.72	3.08	14.72	3.08	11780	6.59	394.8	67.8	10.52	3.93	0.01
11827	17Ti/SBA-15	0.00	0.00	17.06	3.56	17.06	3.56	11780	6.49	364.7	54.2	10.47	3.98	0.03
11836	19Ti/SBA-15	0.00	0.00	19.16	4.00	0.00	4.00	11780	6.38	307.9	45.6	10.44	4.06	0.07
11838	20Ti/SBA-15	0.00	0.00	20.25	4.23	20.25	4.23	11780	6.37	302.8	48.9	10.43	4.06	0.07
11840	21Ti/SBA-15	0.00	0.00	21.09	4.41	21.09	4.41	11780	6.18	288.9	31.4	10.39	4.21	0.15
11876	22.5Ti/SBA-15	0.00	0.00	22.50	4.70	22.50	4.70	11780	6.07	280.4	11.9	10.36	4.29	0.19
11886	23Ti/SBA-15	0.00	0.00	23.28	4.86	23.28	4.86	11780	5.96	266.8	15.8	10.36	4.40	0.24

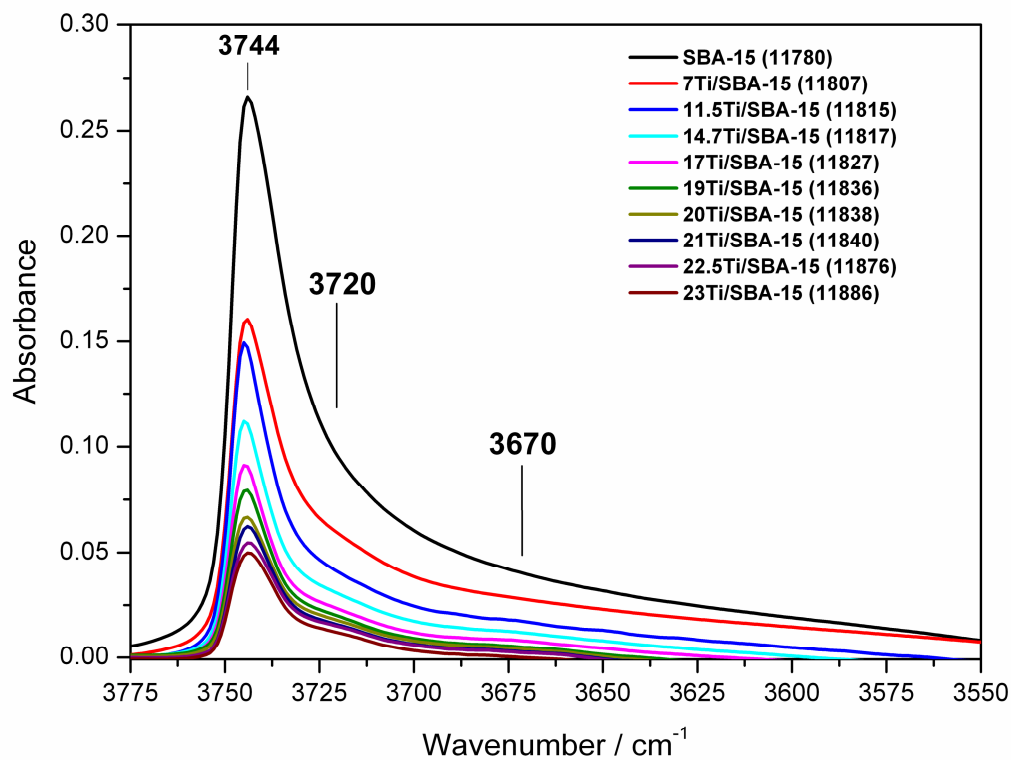
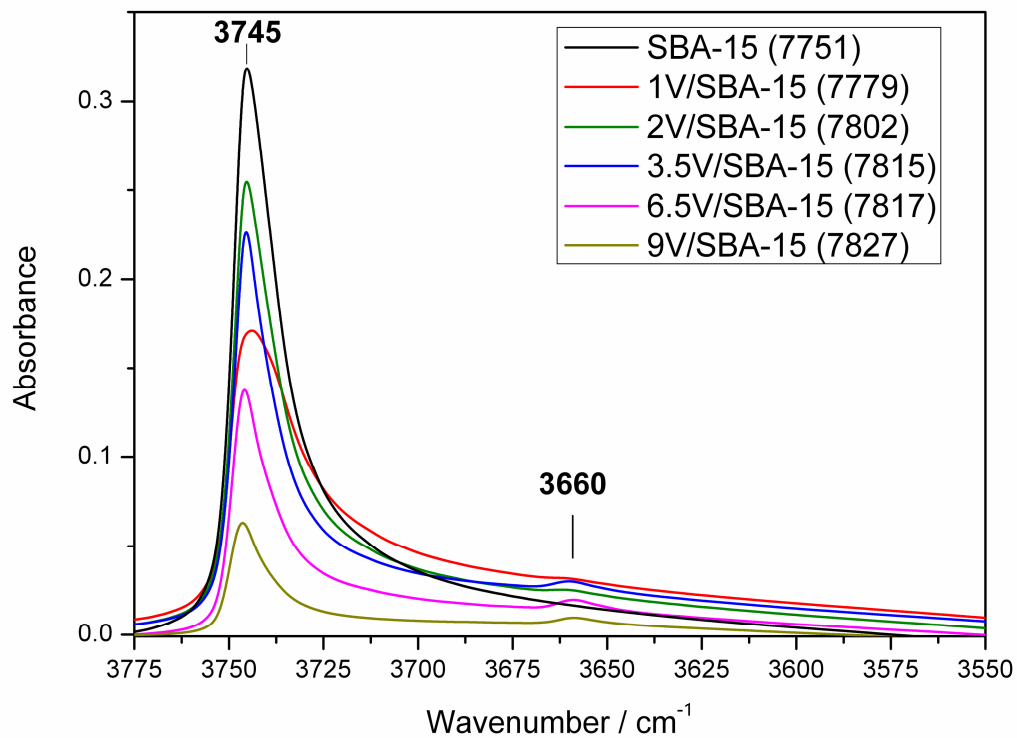
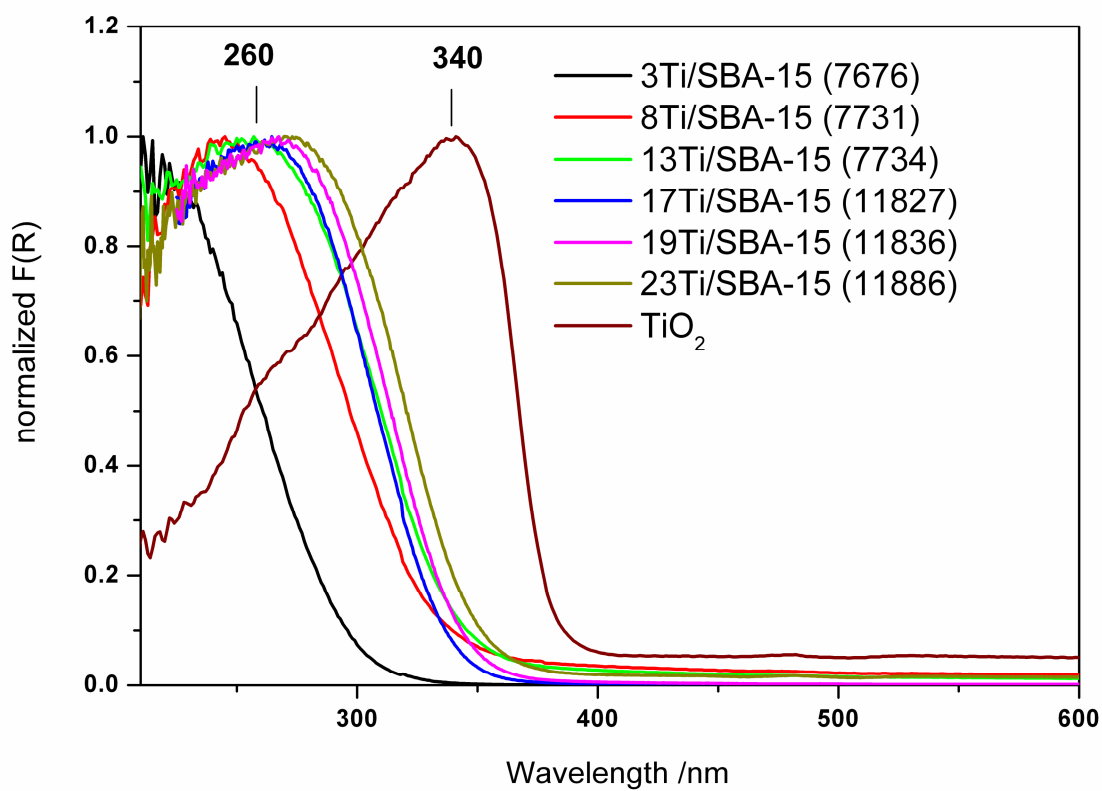


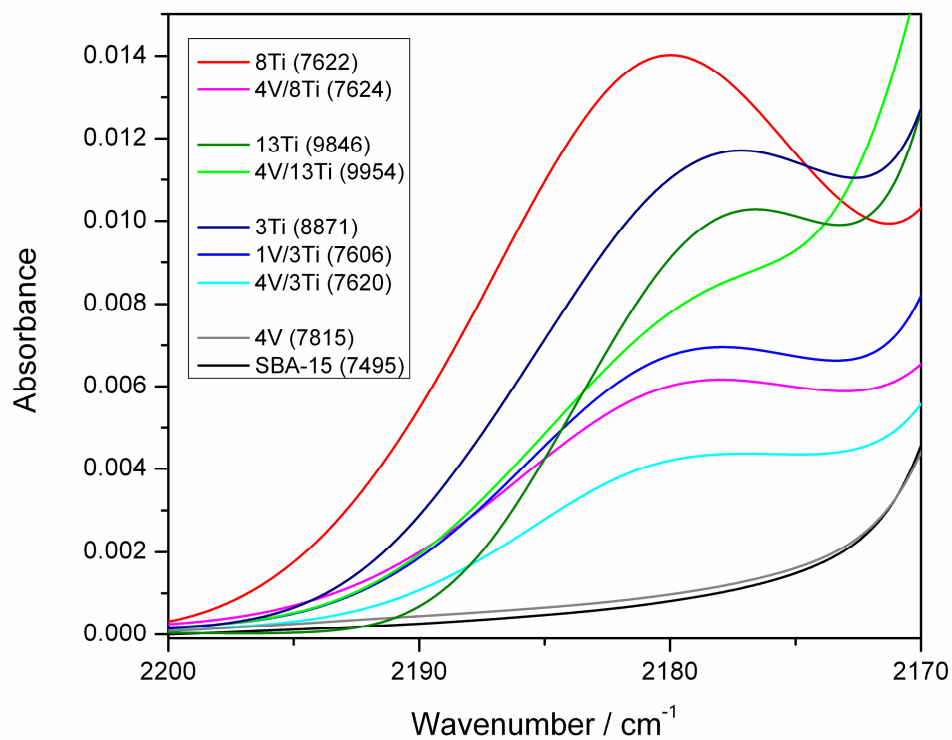
Figure S1: FTIR spectra of selected Ti/SBA-15 catalysts after activation in 200 mbar O₂ at 723 K for a period of 1 h. Spectra are normalized according to areal density of the wafers used. Sample ID numbers are indicated in the figure legend.



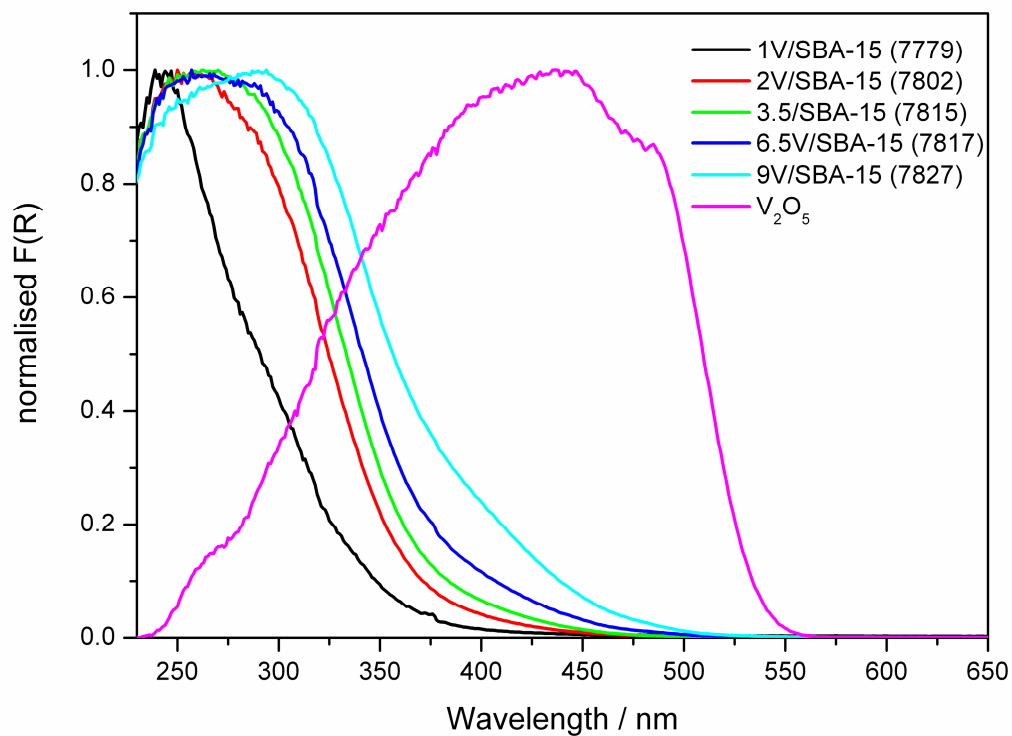
S2: FTIR spectra of selected V/SBA-15 catalysts after activation in 200 mbar O_2 at 723 K for a period of 1 h. Spectra are normalized according to areal density of the wafers used. Sample ID numbers are indicated in the figure legend.



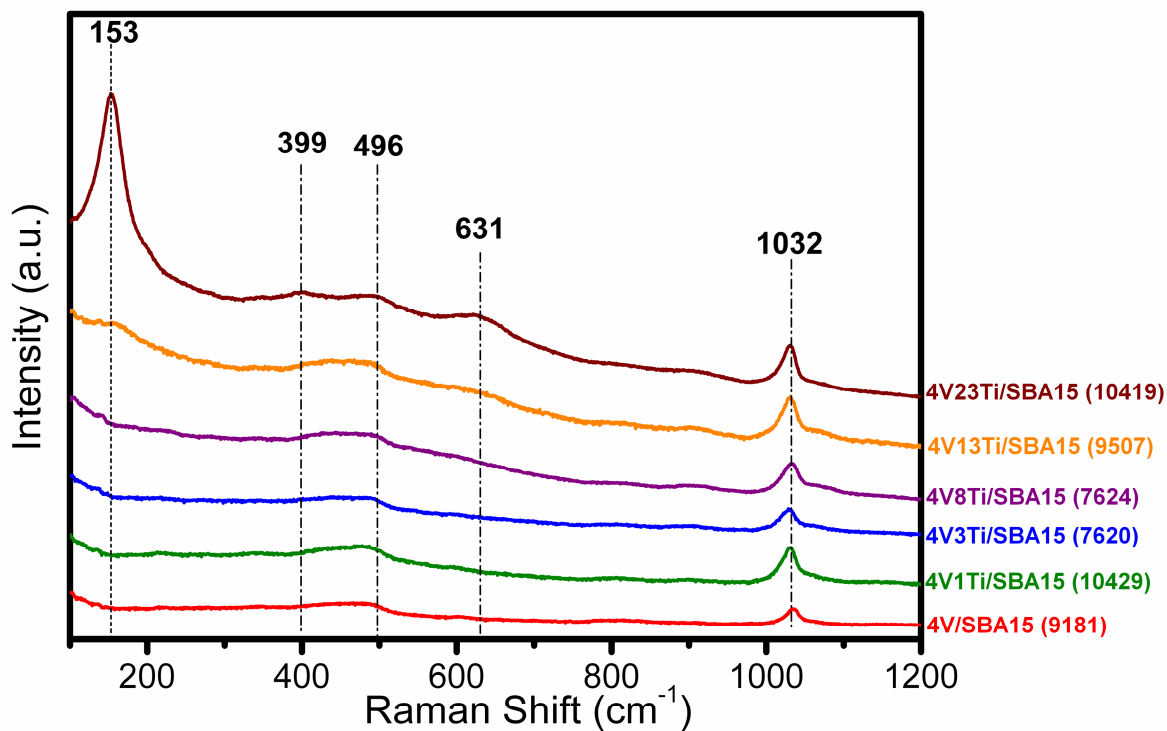
S3: Diffuse reflectance UV-vis spectra of selected Ti/SBA-15 samples after activation in flowing synthetic air at 723 K for a period of 1 h. Sample ID numbers are indicated in the figure legend.



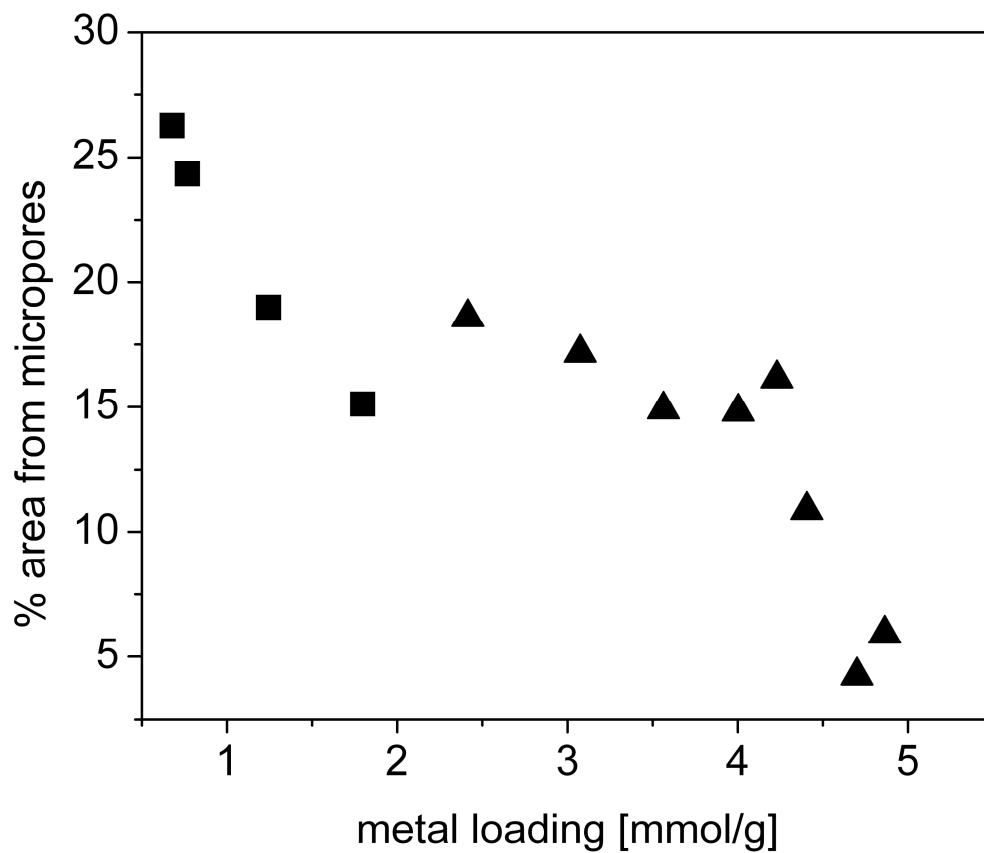
S4: FTIR spectra of CO adsorbed on various $(\text{TiO}_x)_n/\text{SBA-15}$, $(\text{VO}_x)_n/\text{SBA-15}$, and $(\text{VO}_x)_n$ - $(\text{TiO}_x)_n/\text{SBA-15}$ catalysts in the $\nu_{C=O}$ region. Sample ID numbers are indicated in the figure legend.



S5: Diffuse reflectance UV-vis spectra of selected V/SBA-15 samples after dehydration in flowing synthetic air at 723 K for a period of 1 h. Sample ID numbers are indicated in the figure legend.



S6: Raman spectra of catalysts with 4 wt% vanadium with varying titanium content. Spectra were collected using 532 nm laser excitation source (Coherent Compass 315M-150, Nd:YAG double diode) with a power of 10 mW measured at the sample. Samples were located in an *in-situ* cell (Linkam TS1500) before being dehydrated at 723 K in flowing synthetic air for a period of 1 h. All spectra acquired at room temperature. Sample ID numbers are indicated in the figure legend.



S7: Percentage contribution of microporosity to total specific surface area of V/SBA-15 (filled squares) and Ti/SBA-15 (filled triangles) catalyst samples as determined by t-plot analysis.