Supplementary Information

Design, Synthesis and Catalytic Performances of Vanadium-incorporated Mesoporous Silica KIT-6 Catalysts for the Oxidative Dehydrogenation of Propane to Propylene

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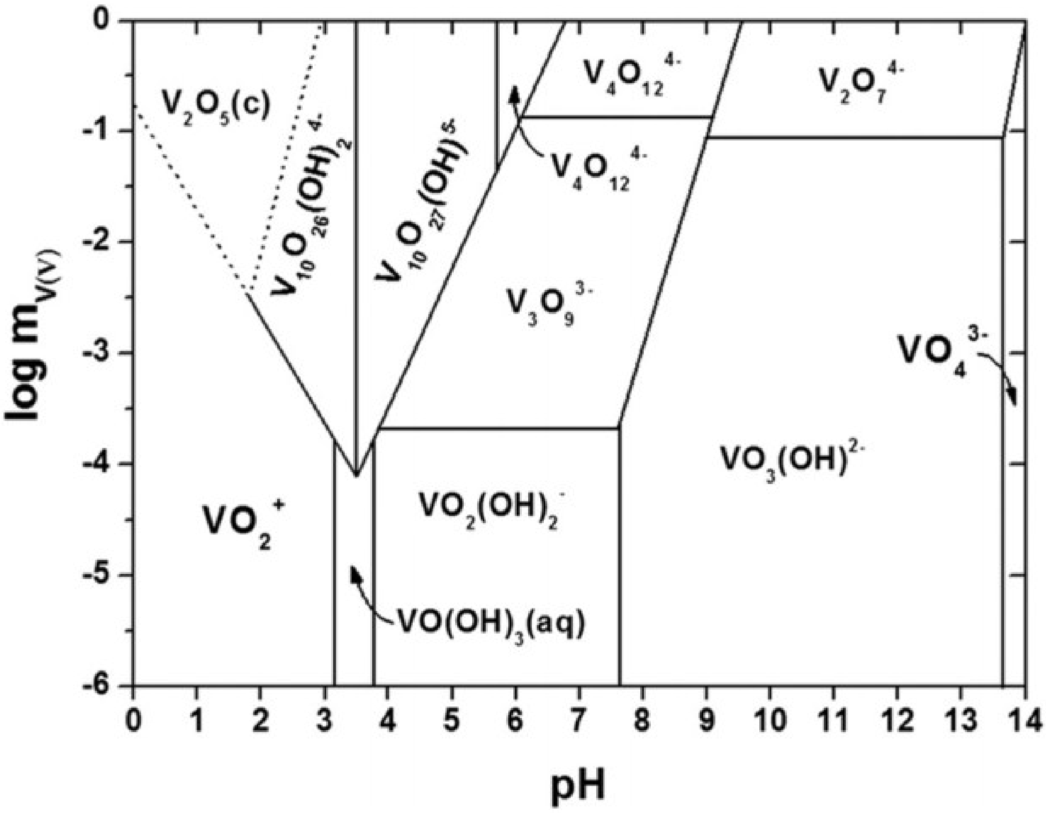

Fig. S1 Aqueous phase equilibrium chemistry of vanadium oxide as a function of both the concentration of vanadium and pH of the solution.[1,2]

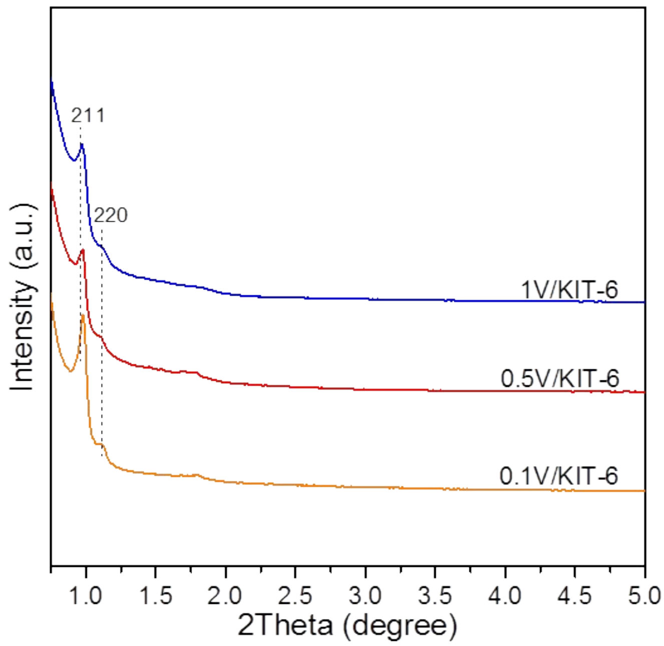

Fig. S2 Low-angle XRD patterns of V/KIT-6 samples.

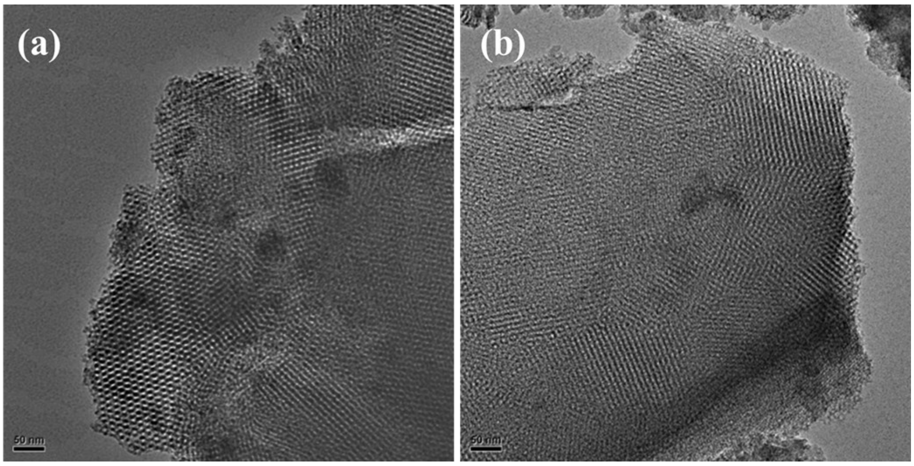

Fig. S3 TEM images of V/KIT-6 samples: (a) 0.5V/KIT-6, (b) 1V/KIT-6.

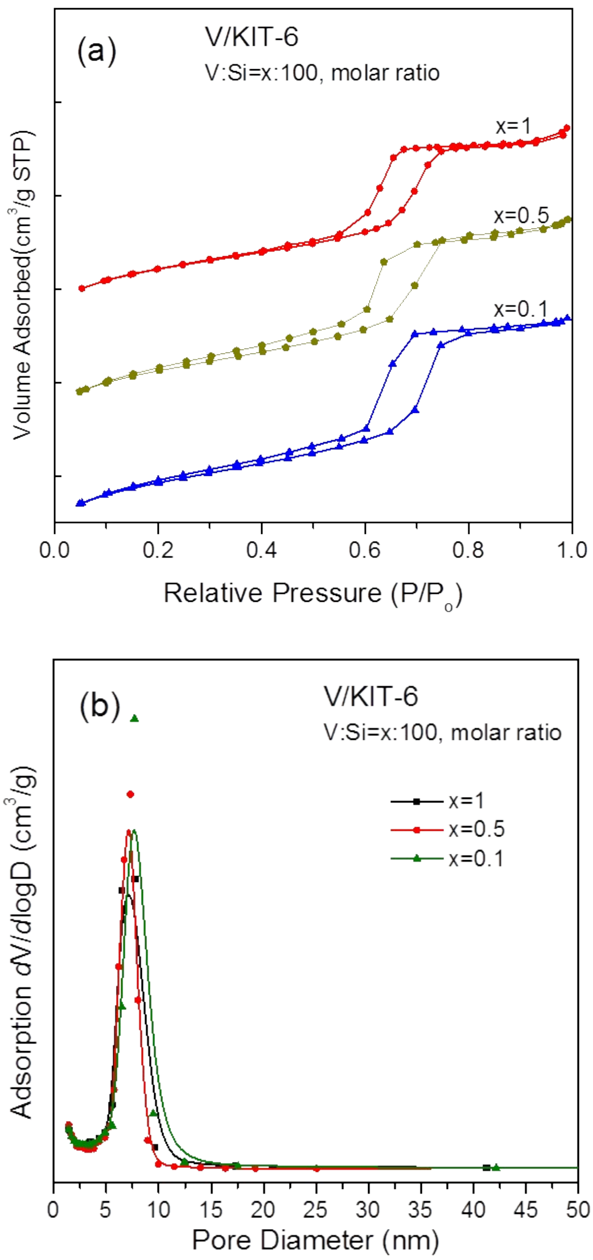

Fig. S4 (a) The N_2 adsorption-desorption isotherms and (b) pore-size distribution of V/KIT-6 samples.

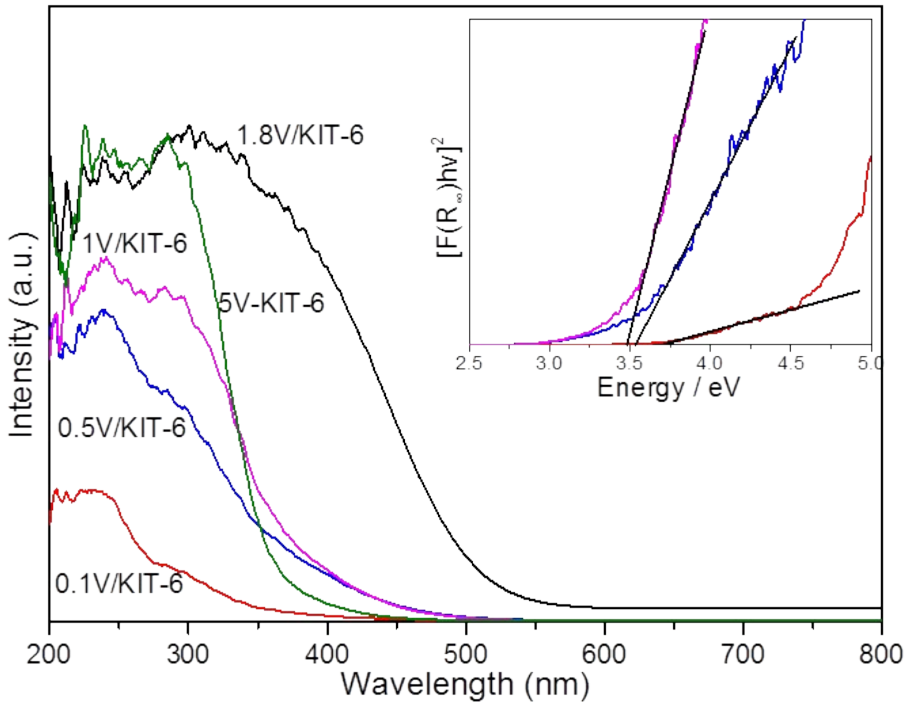

Fig. S5 UV-Vis diffuse reflectance spectra of 5V-KIT-6 and V/KIT-6 samples with different V contents. Inset shows least-squares fits of a line through the low edge energy of the transformed spectra.

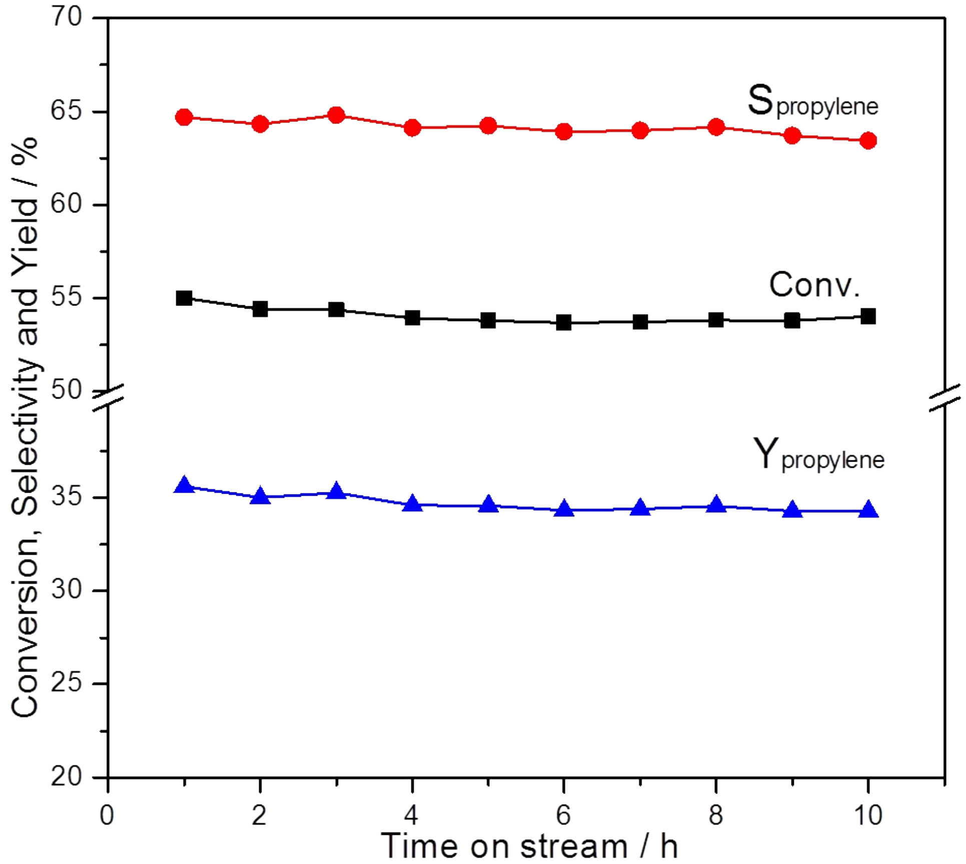

Fig. S6 C_3H_8 conversion, C_3H_6 selectivity and yield as a function of reaction time for ODH of propane over 5V-KIT-6 catalyst. Reaction conditions: catalyst weight = 0.10 g, T=600 °C, $C_3H_8/O_2/N_2$ = 1/1/8, flow rate = 40.0 mL min^{-1}.

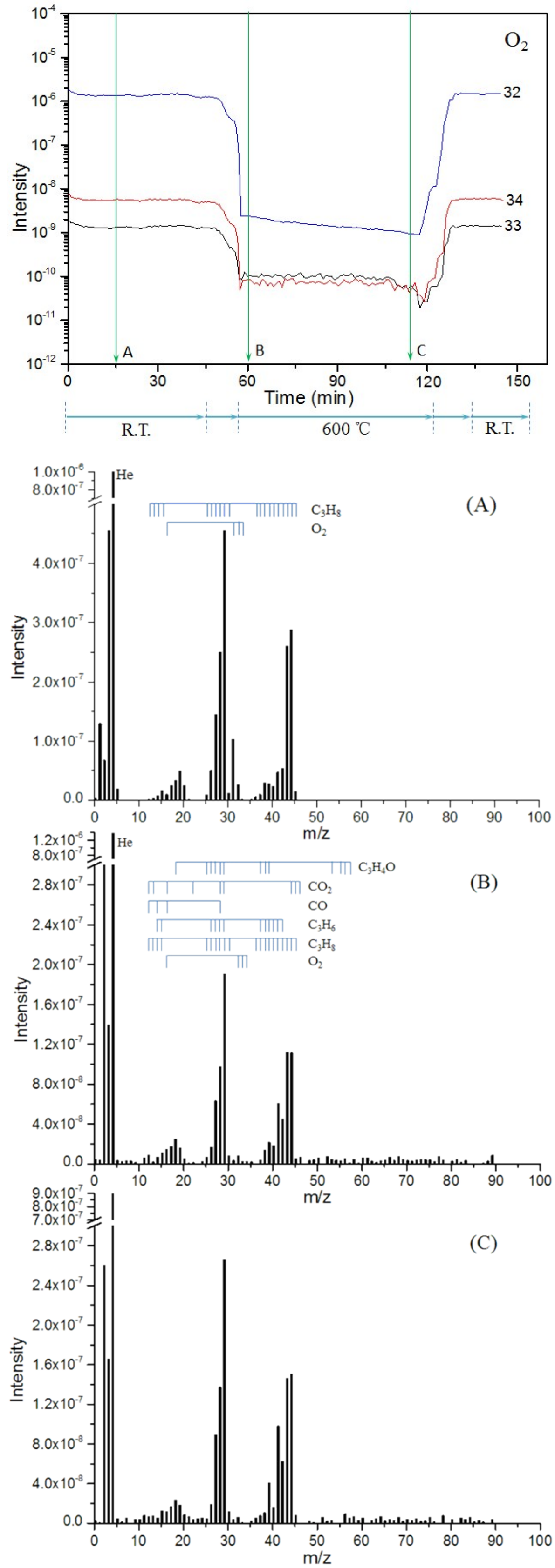

Fig. S7 MS spectra of the components in the reaction mixture for the ODH of propane over 5V-KIT-6 catalyst and the standard samples from the MS library. (A) before reaction, (B) reacting at 600 ^{o}C, (C) after 1 h reaction at 600 ^{o}C.

Table S1 Physico-chemical properties of V/KIT-6 samples.

Samples	V:Si (molar ratio in recipe)	V:Si[a] (final molar ratio)	S_{BET}[b] (m^2/g)	V_P[c] (cm^3/g)	D[d] (nm)	d_{211}	a_0[e] (nm)	δ[f] (nm)	E_g[g] (eV)
0.1V/KIT-6	0.10:100	0.12:100	724	0.80	8.0	9.08	22.2	3.1	3.70
0.5V/KIT-6	0.50:100	0.53:100	648	0.75	7.8	9.08	22.2	3.3	3.52
1V/KIT-6	1.00:100	1.04:100	621	0.72	7.8	9.07	22.2	3.3	3.48

[a] V:Si molar ratio measured by XPS. [b] S_{BET} is the specific surface area calculated by BET method. [c] V_P is the total pore volume of pores. [d] D is the pore diameter. [e] XRD unit-cell parameter estimated from the position of the (211) diffraction line ($a_0= 6^{1/2}d_{211}$). [f] the pore wall thickness $\delta=a_0/2-D_p$. [g] E_g is the absorption edge energy.

Table S2. The catalytic performances for the oxidative dehydrogenation of propane over various catalysts [a]

Catalysts	T/°C	Conv./ %	S_{C3H6}/%	Y_{C3H6}/%	STY_{C3H6}/kg kg_{cat}^{-1} h^{-1}	References	Notes
V-KIT-6	600	47.6	59.8	28.5	3.91	This work	
V/SBA-15	600	41.7	57.0	23.8	0.99	3	
V-SBA-15	600	48.6	41.8	20.3	3.35	4	
V/MCF	550	40.8		27.9	3.77	5	
V/Sb/TiO_2	500	25.4	42.6	10.8	2.02	6	
V/MCM-41	550	49.1	17.2	8.6	0.41	7	
Pt/Al_2O_3	400	14.0	37.0	5.2	1.59	8	
V/γ-Al_2O_3	350	23.0	49.1	11.3	10.6	9	
Cr–Al pillared clay	450	26.7	38.0	10.3	0.28	10	
V–Sb–O/SiO_2	600	40.1	65.6	26.3	4.34	11	
Fe-ZSM-5	450	50	44	22	16.5	12	N_2O as the oxidant
P-Nanodiamond	500	~20	~45	~9	-	13	
K-Mo/SiO_2/TiO_2	550	-	-	~30	-	14	
flame-made V_2O_5/SiO_2	550	23.7	33.2	7.9	1.8	15	
V/Ti/SBA-15	500	2-6	-	-	6-9	16	
V/TiO_2	500	30.4	22.8	6.9	1.43	17	

[a] T: Reaction temperature; Conv.: Conversion of propane; S_{C3H6}: Selectivity of propylene; Y_{C3H6}: Yield of propylene; STY_{C3H6}:Space-time yield of propylene.

Table S3 the TOF values for propylene formation over various catalysts for ODH of propane.

Catalyst	V:Si, molar ratio	TOF, s^{-1}	References
0.1V-KIT-6	0.10:100	0.102	this work
5V-KIT-6	1.80:100	0.027	this work
V-MCF	0.15:100	0.078	18
V-MCF	1.08:100	0.028	18
V-SBA-15	1.8:100	0.075	4
V/Ti/SBA-15	4 wt%	~0.076	16
V-SBA-15 (treated by H_2O_2)	~1.76:100	~0.051	19
V/MCF	~3.29:100	0.026	5
V/SBA-15	~3.29:100	0.026	5
V/SBA-15	~1.18:100	~0.0036	3
V-HMS	~1.41:100	0.0012	20
V_2O_5/SiO_2 (flame-made)	~0.49:100	0.018	15
V/MCM-48	~4.24:100	0.0020	21
V/SBA-16	~4.24:100	0.0019	21
Pt ALD	-	0.43±0.04	8

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