Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Design, synthesis and catalytic performance of vanadium-incorporated mesoporous silica with 3D mesopore structure for propene epoxidation

Agnieszka Held*, Ewa Janiszewska*, Justyna Czerepińska, Jolanta Kowalska-Kuś

Adam Mickiewicz University, Faculty of Chemistry, Uniwersytetu Poznańskiego 8, 61-614 Poznan, Poland

Keywords: propene, epoxidation, mesoporous vanadosilicates, N_2O, hydrothermal synthesis

**Author to whom correspondence should be addressed*

E-mail: awaclaw@amu.edu.pl (A. Held), eszym@amu.edu.pl (E. Janiszewska)

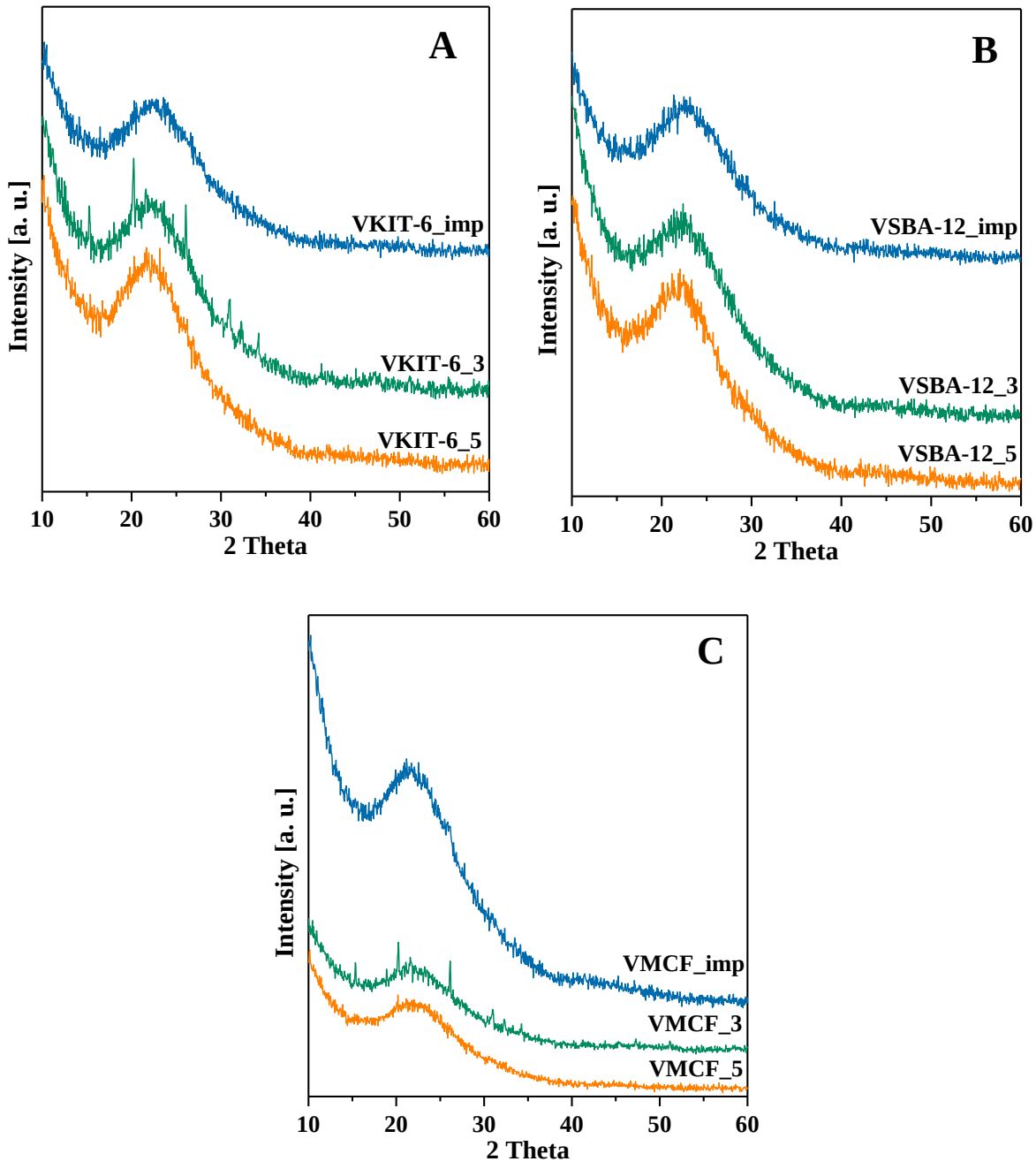

Fig. 1S Wide-angle XRD patterns of V-containing catalysts.

Table 1S Results of the UV-vis spectra data for V-containing catalysts.

Sample	Distribution of V-species			
	$V^{\delta+}$ inside wall	$V^{\delta+}$ on wall surface	$V^{\delta+}$ in external clusters	
	< 250 nm	~250-300 nm	[%]	
	[%]	[%]	300 - 350nm	>350nm
VMCF_3	11.5	1.5	65.2	21.8
VMCF_5	27.7	32.1	20.2	20.0
VMCF_imp	35.9	52.6	0	11.5
VSBA-12_3	45.7	13.5	31.9	8.9
VSBA-12_5	40.2	50.8	9.0	0
VSBA-12_imp	25.2	30.9	0	43.9
VKIT-6_3	25.7	13.2	52.4	8.6
VKIT-6_5	24.3	32.7	29.5	13.5
VKIT-6_imp	28.8	55.0	0	16.2

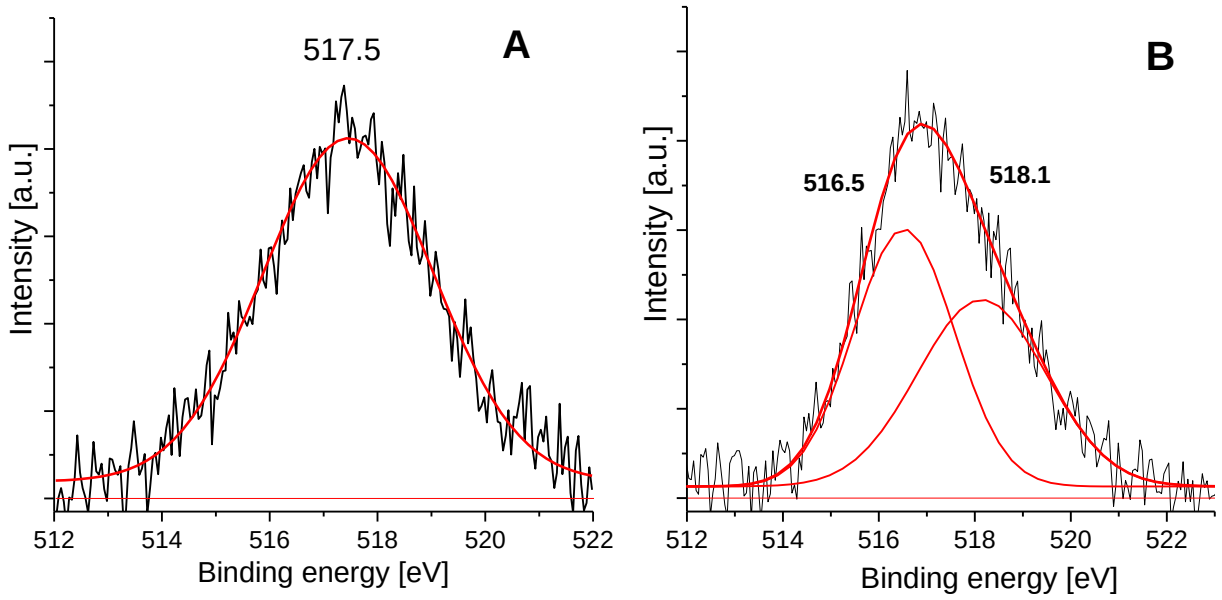

Fig. 2S Deconvoluted XPS V $2p_{3/2}$ spectra of the impregnated VMCF_imp (A) and synthesized VMCF_3 (B) samples.

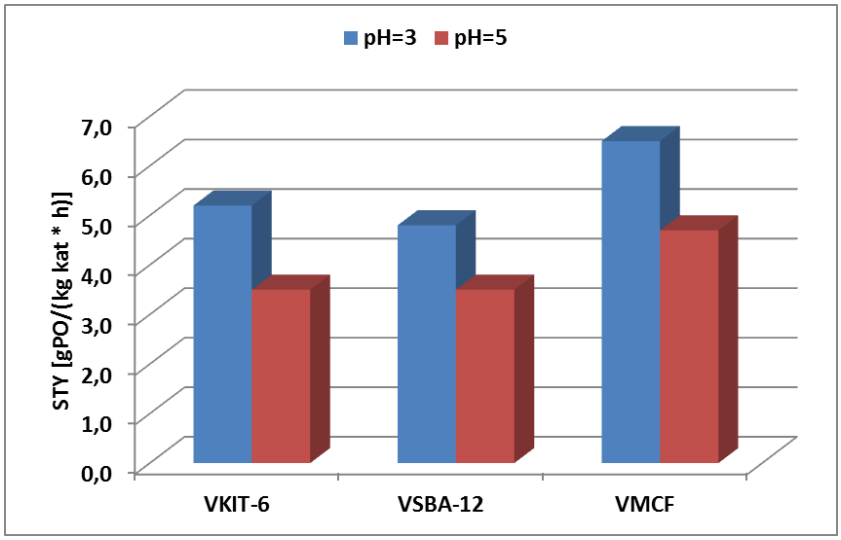

Fig. 3S Space time yield (STY) of propene oxide over vanadium modified mesoporous silica synthesized at different pH; reaction temperature 653K.

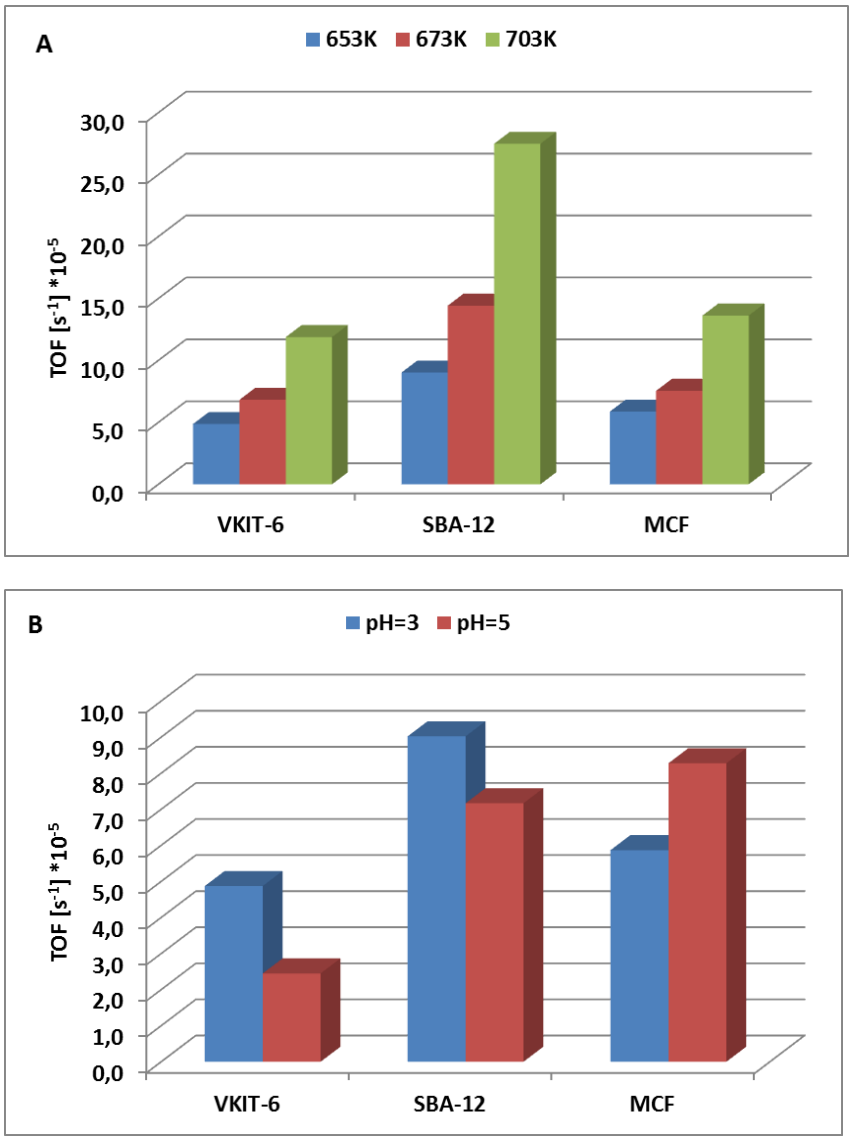

Fig. 4S Comparison of specific activity expressed as turnover frequency (TOF) for propene epoxidation towards propene oxide on VKIT-6, VSBA-12, and VMCF: (A) samples synthesized at pH=3; (B) samples synthesized at different pH (reaction temperature 653K).

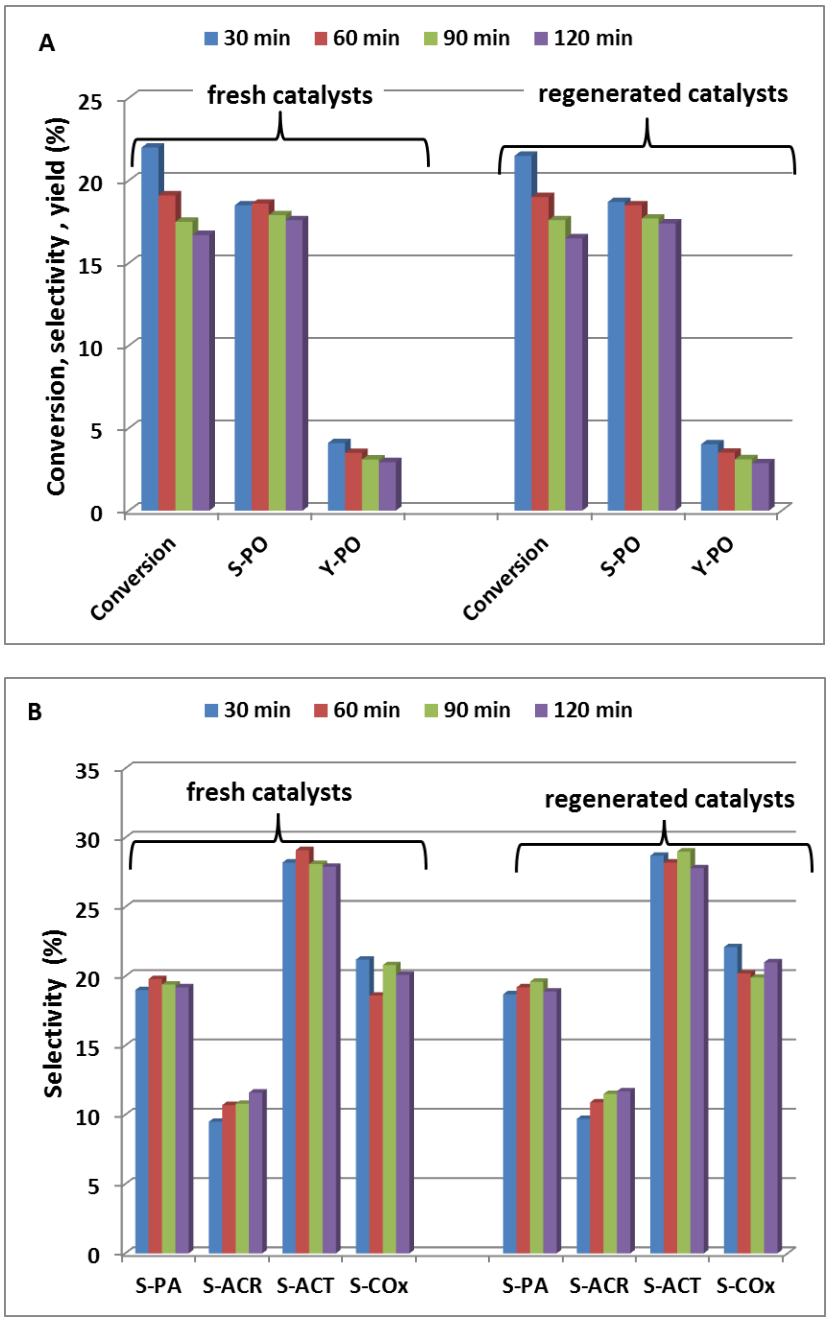

Fig. 5S Catalytic activity of fresh and regenerated VKIT-6_3, tested at 703K within 2 hours, expressed as propene conversion, selectivity to PO, PO yield (A) and selectivity to other oxygen-bearing products (B).

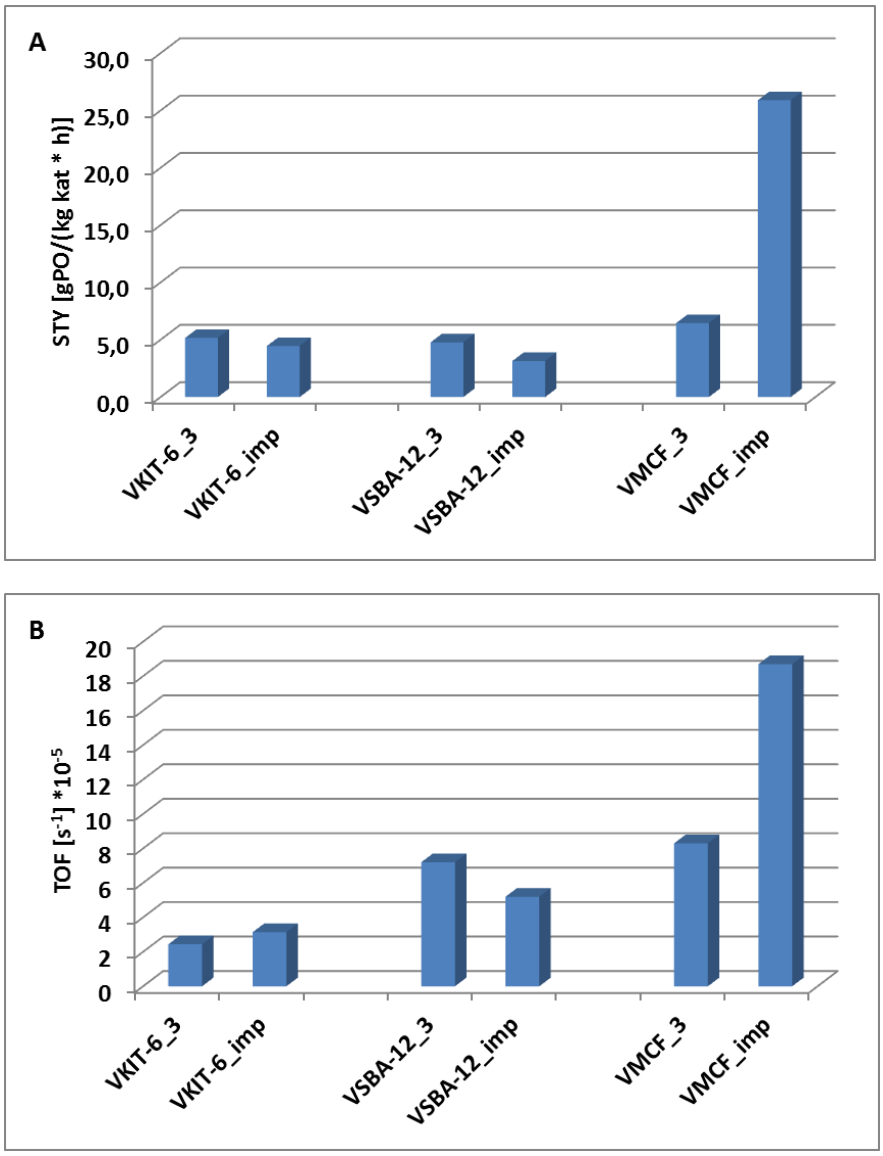

Fig. 6S Comparison of catalytic activity of VKIT-6, VSBA-12, and VMCF samples prepared by direct synthesis at pH=3 and by impregnation method expressed as space time yield (STY) of PO (A) and turnover frequency (TOF) (B); reaction temperature 653K