The evolution of the M1 local structure during preparation of VMoNbTeO catalyst for ethane oxidative dehydrogenation to ethylene

Kardash T.Yu.[*a], Lazareva E.V.[a], Svintsitskiy D.A.[a], Bondareva V.M.[a] and Neder R.B.[b]*

a - Boreskov Institute of Catalysis SB RAS, Russia, 630090, Novosibirsk, Pr. Ak. Lavrentieva, 5.

b - Friedrich-Alexander University of Erlangen-Nuremberg, Germany, 91058 Erlangen, Staudtstr. 3.

Corresponding author: kardash@catalysis.ru

Supplementary materials:

Table S1. The structural parameters of the crystalline M1 phase calculated from the Rietveld fit

Chemical composition	$(TeO)_{0.39}(V_{1.1}Mo_{3.5}Nb_{0.4})O_{14}$
Space Group	Pba2 (32)
Cell parameters	a = 21.156(2) b = 26.663(4) c = 4.018(5)
Degree of crystallinity	80%
Particle size (CSD), nm	60(2)
Rwp, %	6.2

Table S2. *Surface ratios of elements for studied VMoTeNb samples based on XPS data.*

	D1	H310	H350	H400	H450	H500	H550
V/Mo	0.42	0.22	0.28	0.25	0.27	0.25	0.24
Nb/Mo	0.09	0.09	0.09	0.09	0.10	0.10	0.11
Te/Mo	0.34	0.30	0.29	0.30	0.31	0.31	0.37
O/Mo	7.7	5.9	5.8	5.7	5.6	5.4	5.8
C/Mo	4.5	2.4	2.3	2.5	2.0	1.6	1.6

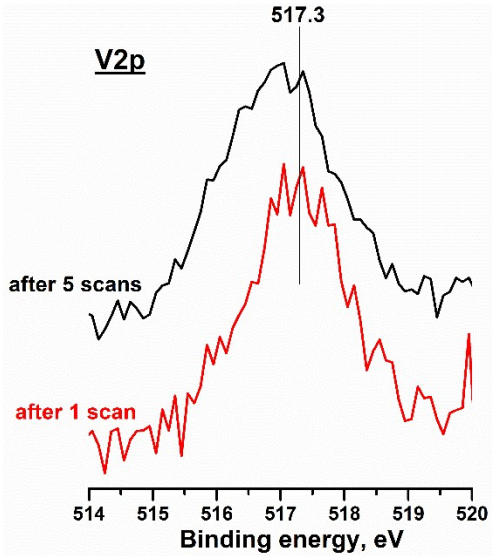

Figure S1. Evolution of V2p spectrum for the spray-dried precursor of VMoNbTe oxide during XPS acquisition.

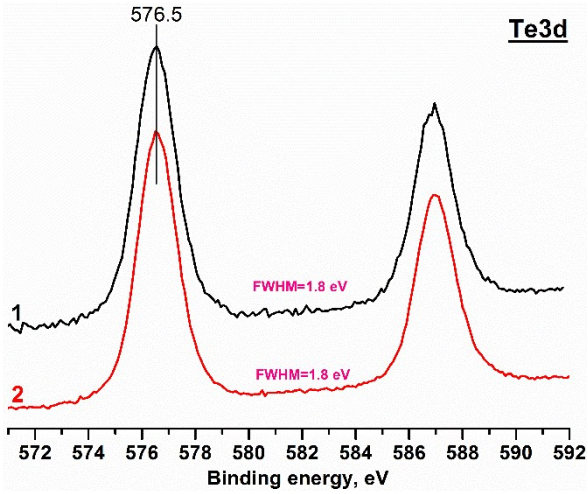

Figure S2. Te3d spectra for VMoNbTe mixed oxide in the form of: 1 – slurry after spray-drying (dry precursor); 2 – dry precursor after thermal treatment in He at 550ºC.

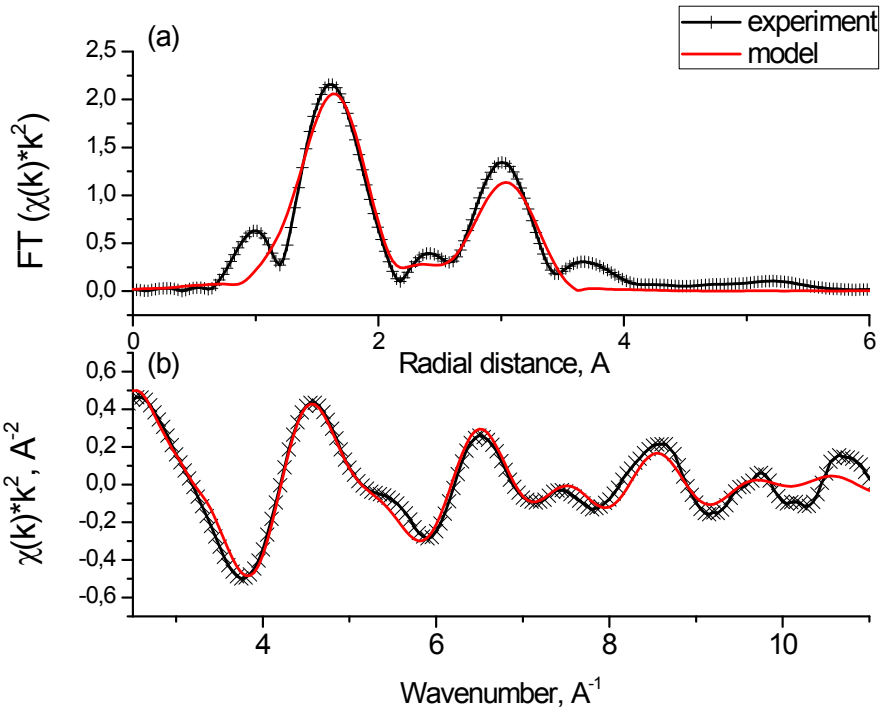

Figure S3. Fourier transform (a), Nb K-edge k²-weighted EXAFS spectra (b) and fits of the spray-dried slurry; experimental data is shown with crossed line, fits – solid line.

Table S3 Nb K-edge fitting results for the spray-dried slurry. R-factor=0.04; S_0^2=0.33(1)

Shell	Coordination number	R, Å	σ^2, Å^{-2}
O	6	2.12(1)	0.009(25)
Nb	2	3.38(2)	0.013(1)