Supporting information

MIL-47(V)-Derived Carbon-doped Vanadium Oxide for Selective Oxidation of 5-Hydroxymethylfurfural to 2,5-Diformylfuran

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Theoretical results: Calculations were performed using spin-polarized Kohn-Sham density functional theory (DFT). We used the generalized gradient approximation with the Perdew-Burke-Ernzerhof[1] exchange-correlation functional as implemented in the Vienna *ab initio* simulation package (VASP).[2,3] The valence orbitals of V (3d, 4s), O (2s, 2p) and C (2s, 2p) were described by plane-wave basis sets with cutoff energies of 400 eV. The Gaussian smearing method with a width of 0.20 eV was used. According to the experimental characterization results, a unit cell of V_2O_5 with a space group of Pmmn was used to model the catalyst structure. Bulk optimization yielded lattice parameters of a =3.56 Å, b=11.51 Å, c=4.36 Å, which were in good agreement with the experimental values. The Brillouin zone was sampled at $(2 \times 2 \times 1)$ and the Γ-point for the calculations. The convergence criteria for the energy and force were set to 10^{-4} eV and 0.03 eV/Å. The oxygen vacancy formation energies were calculated according to the equation, $Ef(Vo)=E (defect)-(E_{V2O5}-\mu o)$, $\mu o= 1/2 E(O_2, g)$.

(1) Perdew, J. P.; Burke, K.; Ernzerhof, M. Phys. Rev. Lett. 1996, 77, 3865.
(2) Kresse, G.; Furthmüller, J. Physical Review B 1996, 54, 11169.
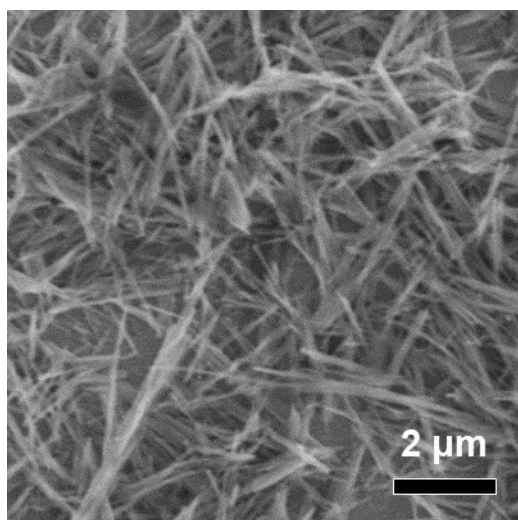(3) Kresse, G.; Furthmüller, J. Computational Materials Science 1996, 6, 15.
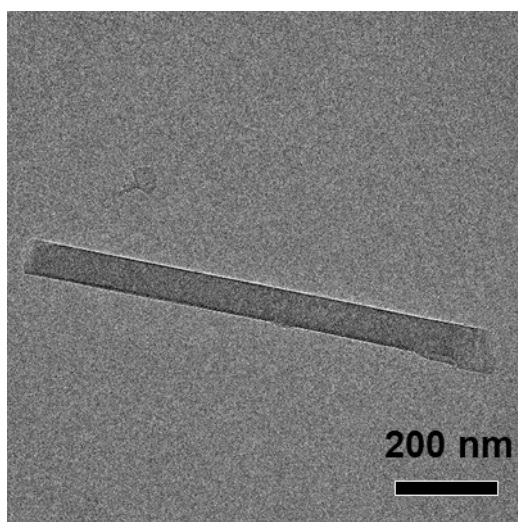
Fig. S1. SEM image of MIL-47 nanorods.

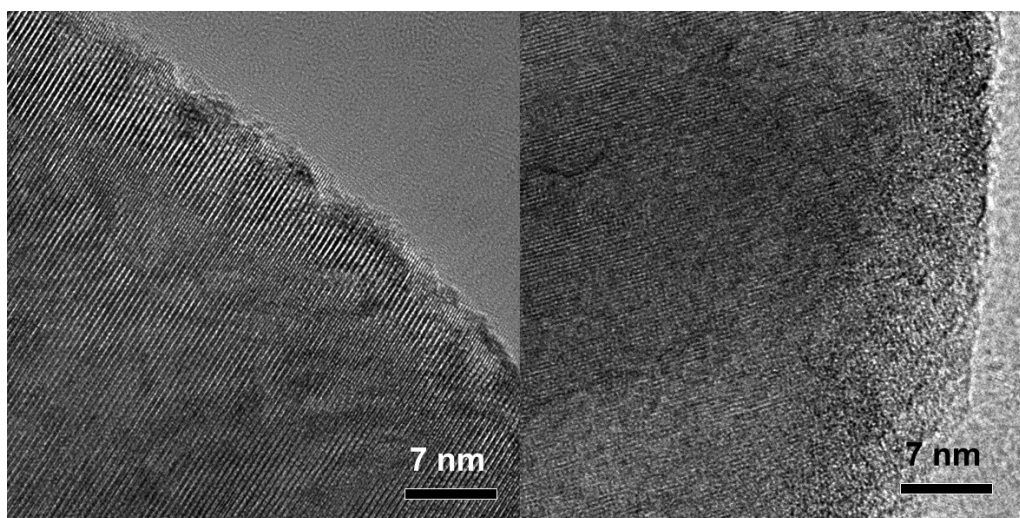**Fig. S2.** HRTEM image of a single MIL-47 nanorod.

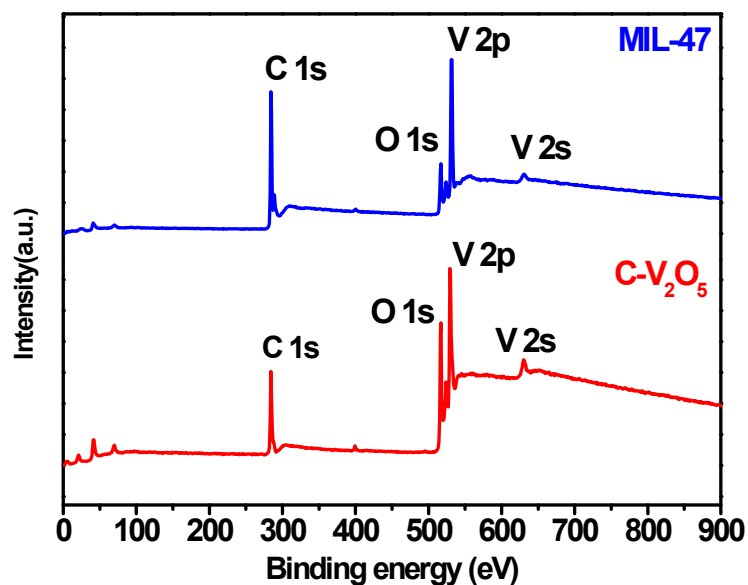**Fig. S3.** HRTEM of C-V_2O_5 at different areas.

Fig. S4. The XPS spectra of MIL-47 and C-V$_2$O$_5$.

Table S1. The area fraction of different V species in MIL-47.

Species	Lines	Position (eV)	Area fraction (%)
V^{5+}	2p$_{3/2}$	517.4	34
	2p$_{1/2}$	524.8	17
V^{4+}	2p$_{3/2}$	516.7	16
	2p$_{1/2}$	523.9	8
V^{3+}	2p$_{3/2}$	515.7	16
	2p$_{1/2}$	523.1	8

Table S2. The area fraction of different V species in C-V$_2$O$_5$.

Species	Lines	Position (eV)	Area fraction (%)
V^{5+}	2p$_{3/2}$	517.4	53
	2p$_{1/2}$	524.8	16
V^{4+}	2p$_{3/2}$	516.7	14
	2p$_{1/2}$	523.9	7
V^{3+}	2p$_{3/2}$	515.7	5
	2p$_{1/2}$	523.1	3

Table S3. The semi-quantitative analysis of XPS.

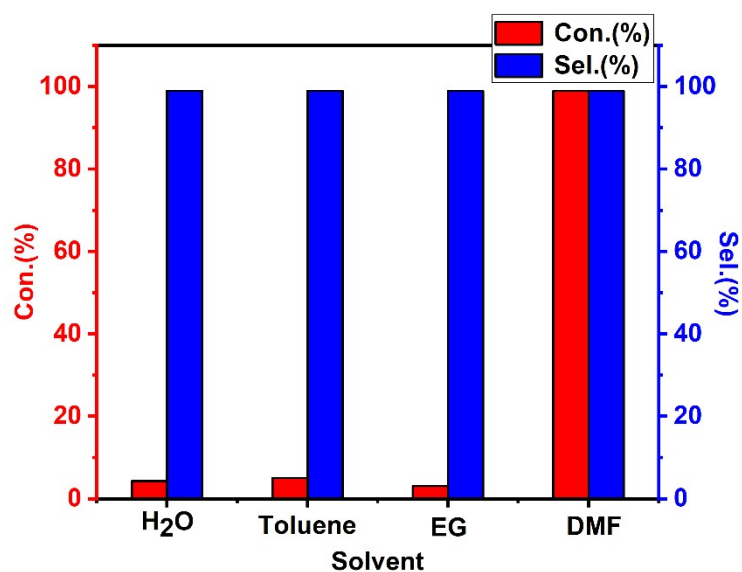| Sample	Element	Atomic F. (%)
MIL-47	C	60.68
	O	26.04
	V	13.29
C-V_2O_5	C	42.09
	O	35.56
	V	22.35

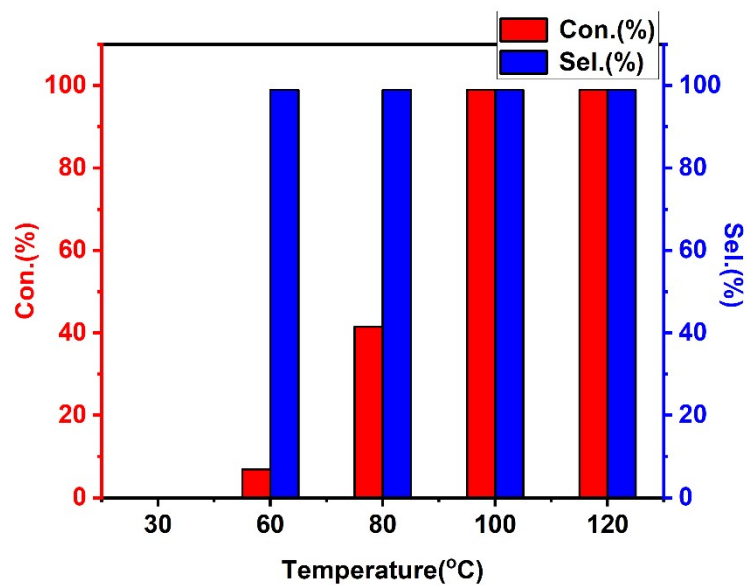**Fig. S5.** Solvent screening of MIL-47 nanorods to HMF oxidation.

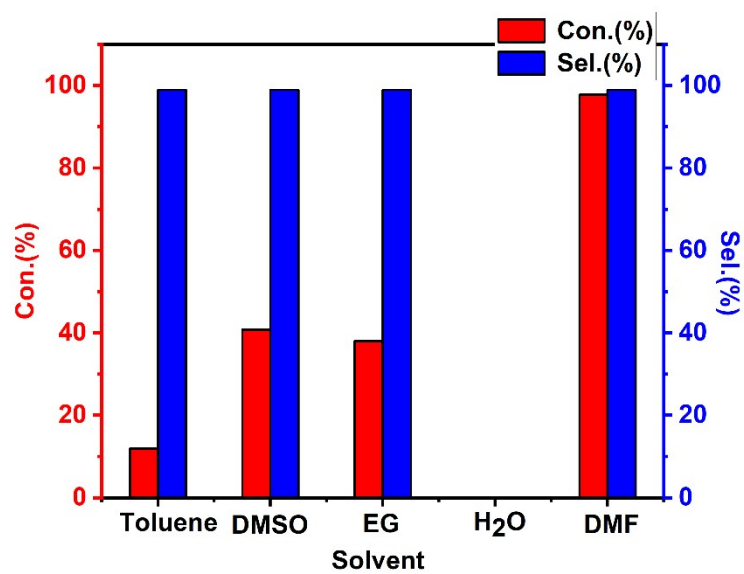**Fig. S6.** The temperature-activity dependence using MIL-47 as the catalyst.

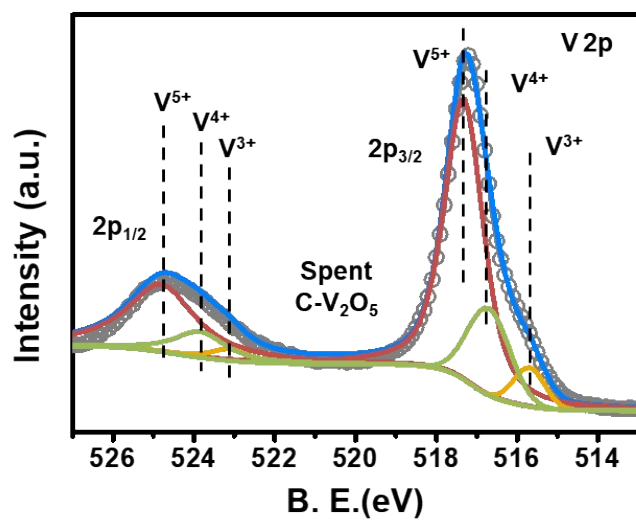**Fig. S7**. Solvent screening of Carbon-V_2O_5 to HMF oxidation.

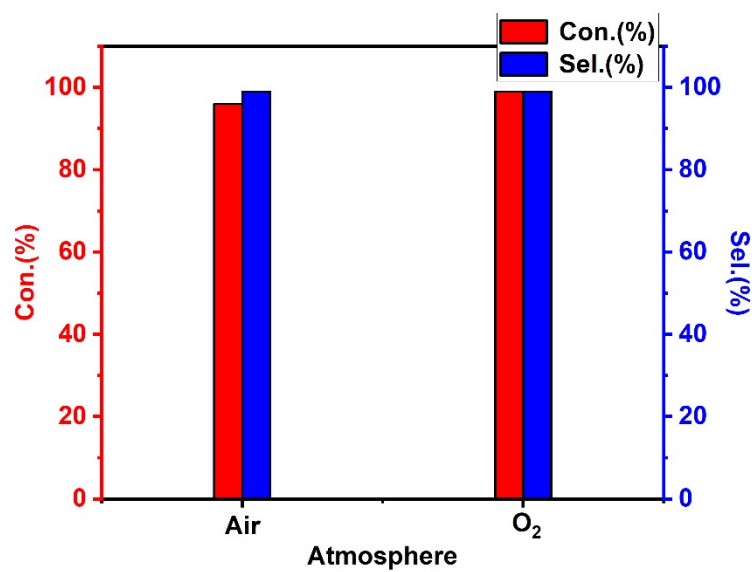**Fig. S8**. The V 2p spectra of spent C-V_2O_5 sample.

Fig. S9. The HMF oxidation is catalyzed by C-V_2O_5 using air or oxygen gas as an oxidant.
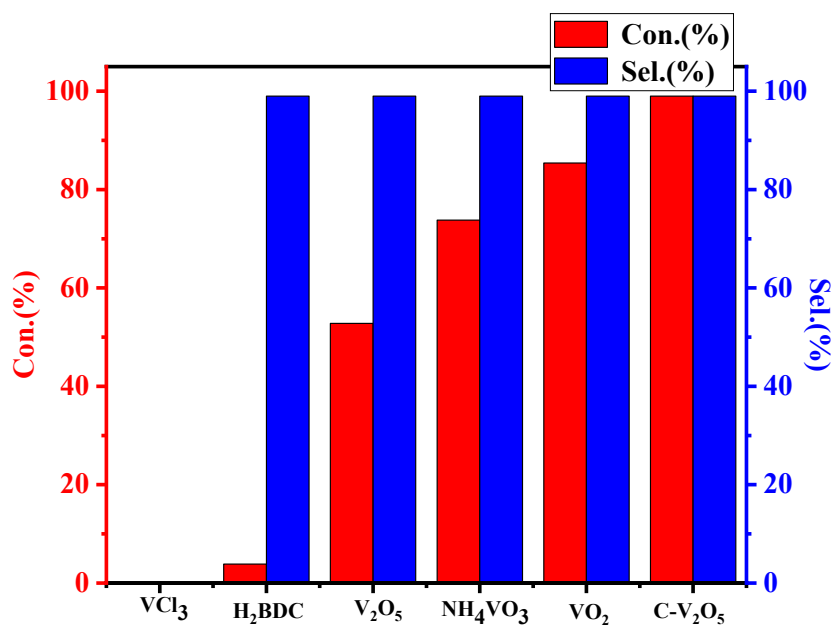

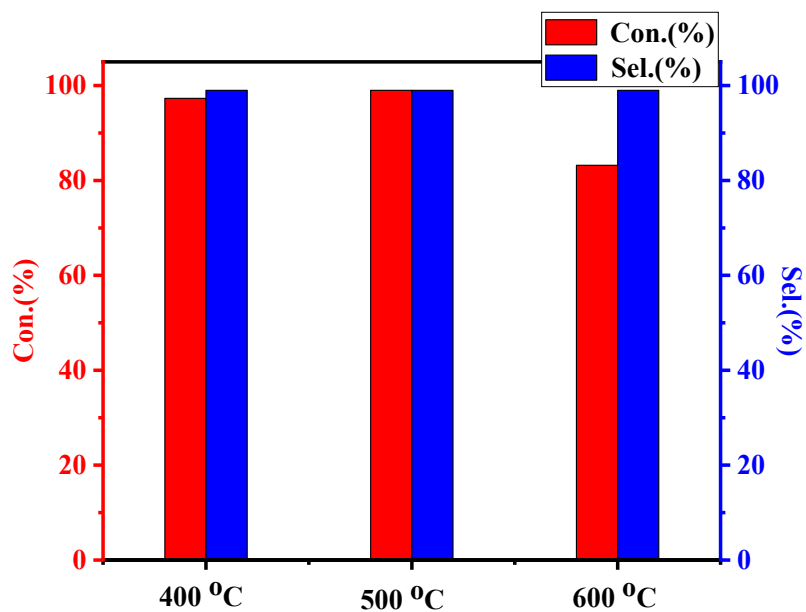**Fig. S10**. The HMF oxidation is catalyzed by different catalysts.

Fig. S11 The HMF oxidation is catalyzed by Catalysts calcined at different temperatures

Table S4. Results of organic element analysis(EA) .

	N(%)	C(%)	H(%)
C-V_2O_5	0.05	0.23	0.101

Table S5. Analysis of metal elements in reaction solution .

	metal	Element concentration of test solution C_0 (mg/mL)
C-V_2O_5	V	0.005481