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Supporting Information

MoO_x-pyridine organic-inorganic hybrid wires as a reusable and highly selective catalyst for the oxidation of alcohols: a comparison study between reaction-controlled phase-transfer catalysis and heterogeneous catalysis

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Table S1 Comparison of the activity of the MoO_x-pyridine wires with other Mo-based catalysts used in oxidation of benzyl alcohol to benzaldehyde with O_2.

Entry	Catalyst	Time (h)	Reaction conditions/T(°C)	Con. (%)	Sel. (%)	Y. (%)	Ref.
1	PVMo/C	22	Toluene/100	97	100	-	[1]
2	$(NH_4)_5H_6PV_8$-Mo_4O_{40}/C	15	Toluene/100	-	-	92	[2]
3	Crystalline Mo–V–O oxide	24	Toluene/80	22	>99	-	[3]
4	TEMPO/$H_5PV_2Mo_{10}O_{40}$	6	Acetone/100	99.6	-	-	[4]
5	$MoO_2(acac)_2$–$Cu(NO_3)_2$	3	Toluene/100	100	98	98	[5]
6	$Q_4[M(dmso)_3Mo_7O_{24}]$ (M=Ru(II), Os(II))	12	Toluene/120	99	99	-	[6]
7	$H_5PV_2Mo_{10}O_{40}$	16	Polyethylene glycol/100	99	100	-	[7]
8	$\{nBu_4N\}_5\{PV_2Mo_{10}O_{40}\}$	15	Benzonitrile/150	100	-	-	[8]
9	$[MoO(O_2)(QO)_2]$	16	Acetonitrile/82	-	-	14	[9]
10	$MoO_2(acac)_n$-NAP-MgO	12	Toluene/110	-	-	81	[10]
11	Polyaniline-supported $MoO_2(acac)_2$	12	Toluene/100	86	>98	-	[11]
12	**MoO_x-pyridine wires**	**0.75**	**Acetic acid/50**	**95**	**100**	**-**	**This work**

Table S2 Comparison of the activity of the MoO_x-pyridine wires with other Mo-based catalysts used in oxidation of benzyl alcohol to benzaldehyde with H_2O_2.

Entry	Catalyst	Time (h)	Reaction conditions/T(°C)	Con. (%)	Sel. (%)	Y. (%)	Ref.
1	$Ph_3P(CH_2)_2PPh_3[MoO(O_2)_2(C_2O_4].2H_2O$	8	Solvent free/90	-	-	93.89	[12]
2	$PPh_4[MoO(O_2)_2(HPEOH)]$	24	Acetonitrile/Reflux	-	-	63	[13]
3	$MoO(O_2)(QO)_2$	16	Acetonitrile/Reflux	-	-	52	[9]
4	$CpMo(CO)_3(C{\equiv}CPh)$	8	Solvent free/80	86	92	79	[14]
5	$[n\text{-}C_4H_9(p\text{-}C_5H_5N)]_4Mo_8O_{26}$	6.5	Solvent free/Reflux	99.5	76.5	-	[15]
6	**MoO_x-pyridine wires**	**0.75**	**Solvent free/80**	**95**	**100**	**-**	**This work**

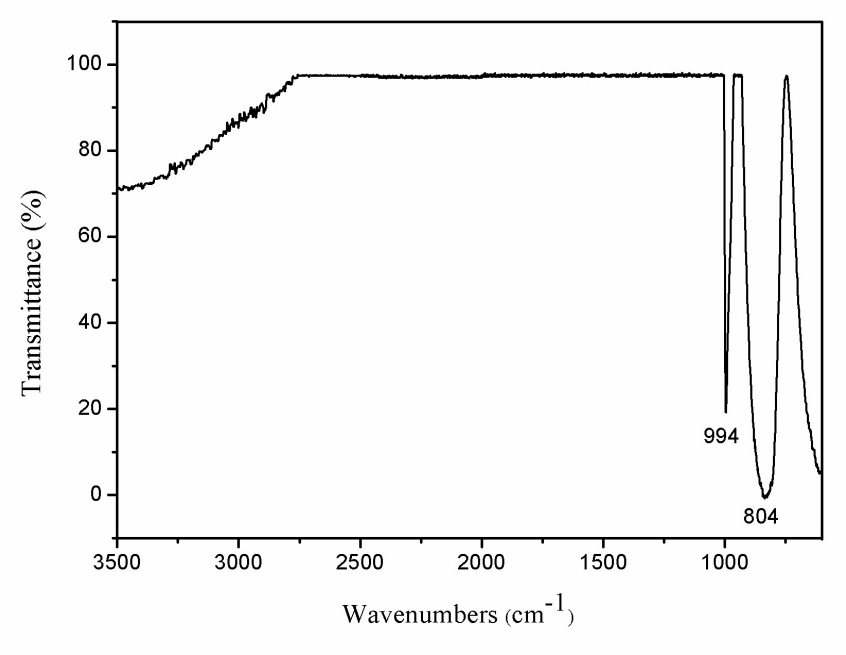

Fig. S1 FT-IR spectrum of the calcined $Mo_3O_{10}(C_5H_6N)_2.H_2O$ wires under air flow for 5 hours at 400 °C.

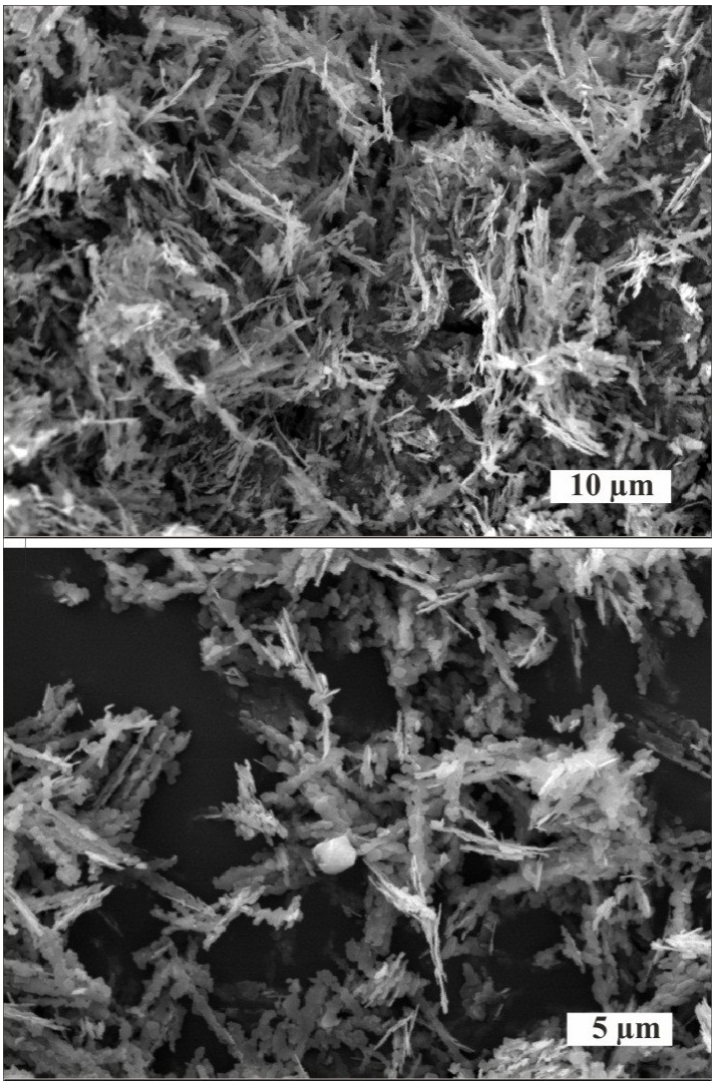

Fig. S2 SEM images of the calcined $Mo_3O_{10}(C_5H_6N)_2.H_2O$ wires under air flow for 5 hours at 400 °C.

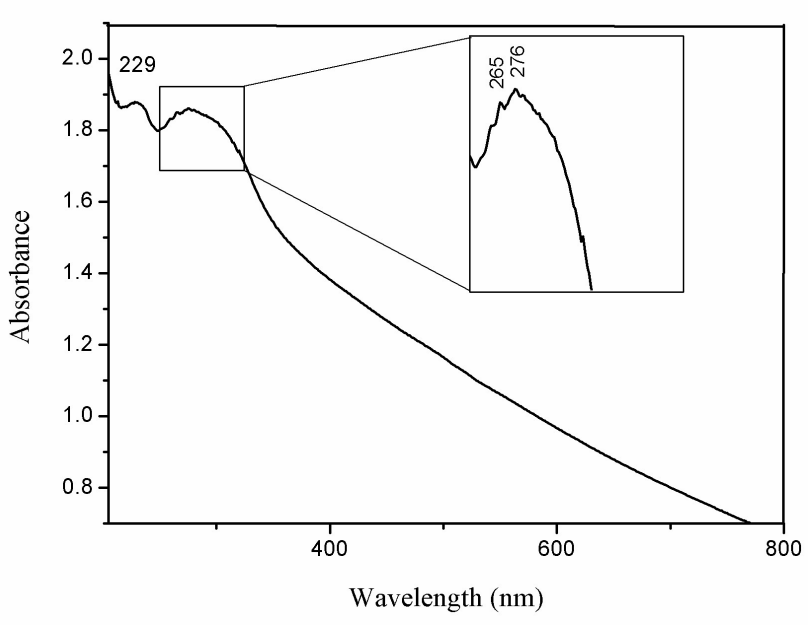

Fig. S3 UV-Vis spectrum of the $Mo_3O_{10}(C_5H_6N)_2.H_2O$ wires. The absorption bands at 229 nm and 265 nm are attributed to LMCT transition ($O^{2-} \rightarrow Mo^{6+}$) and electronic transition of the pyridine ring (π-π*), respectively. In addition, the band in the range of 270-300 nm is the characteristic absorption of the bridging Mo-O-Mo structure [16].

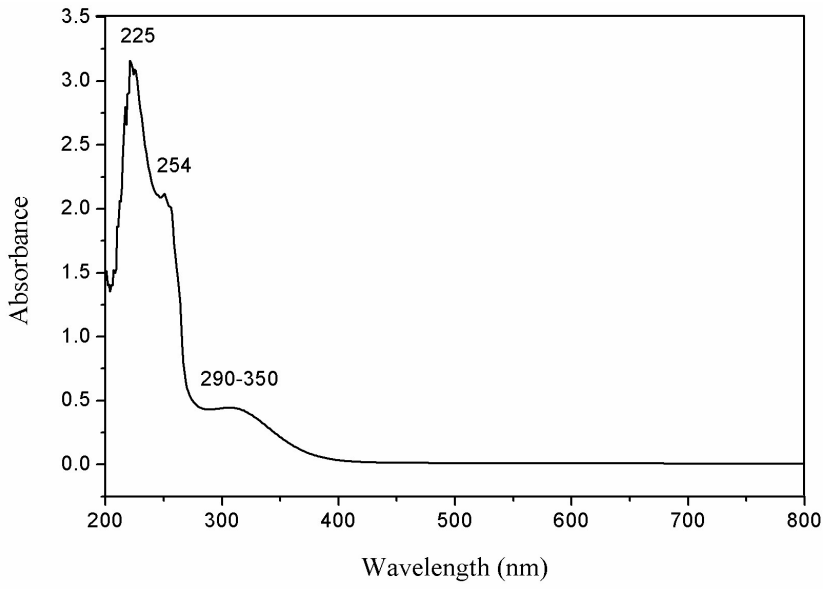

Fig. S4 UV-Vis spectrum of the active catalyst II (during the reaction). LMCT transition ($O^{2-} \rightarrow Mo^{6+}$) and the electronic transition (π-π^*) can be observed at 225 and 254 nm, respectively. The absorption band of the bridging Mo-O-Mo completely is gone and a new peak is appeared in the range of 290-350 nm indicated the presence of peroxo-molybdenum species.

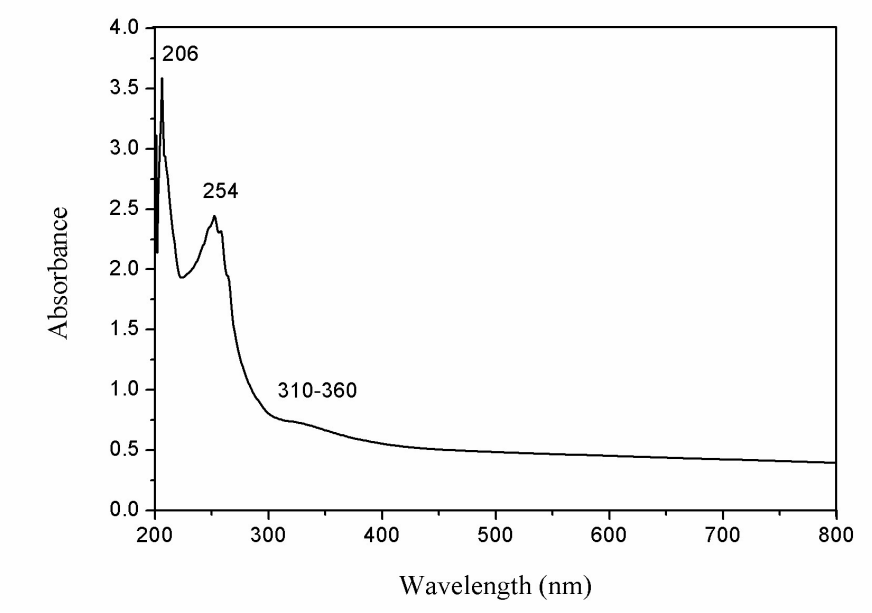

Fig. S5 UV-Vis spectrum of the reused catalyst from the H_2O_2 system. LMCT transition ($O^{2-}\rightarrow Mo^{6+}$) and the electronic transition (π-π^*) can be observed at 206 and 254 nm, respectively. In addition, the broad absorption in the range of 310-360 nm indicated the presence of $O_2^{2-}\rightarrow Mo^{6+}$ electronic transition.

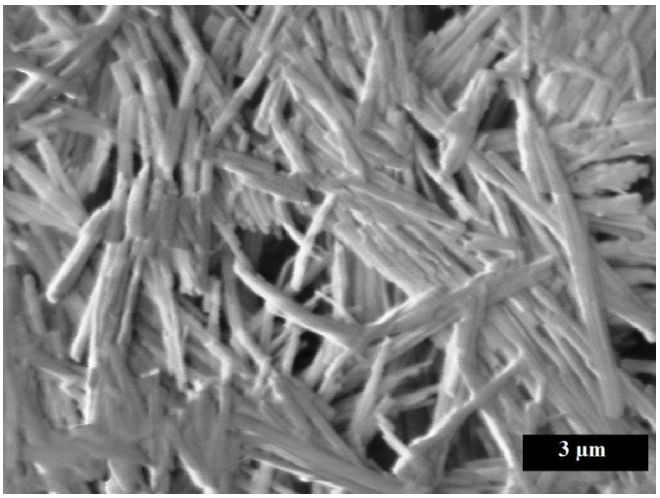

Fig. S**6** SEM image of the reused catalyst from the O_2 system.

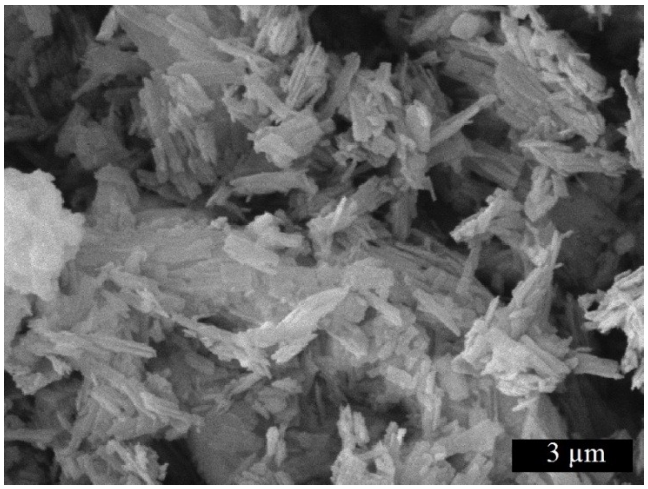

Fig. S**7** SEM image of the reused catalyst from the H_2O_2 system.

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