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Synergy of highly dispersed Pd and oxygen vacancy promoted hydrodeoxygenation of lactic acid to propionic acid

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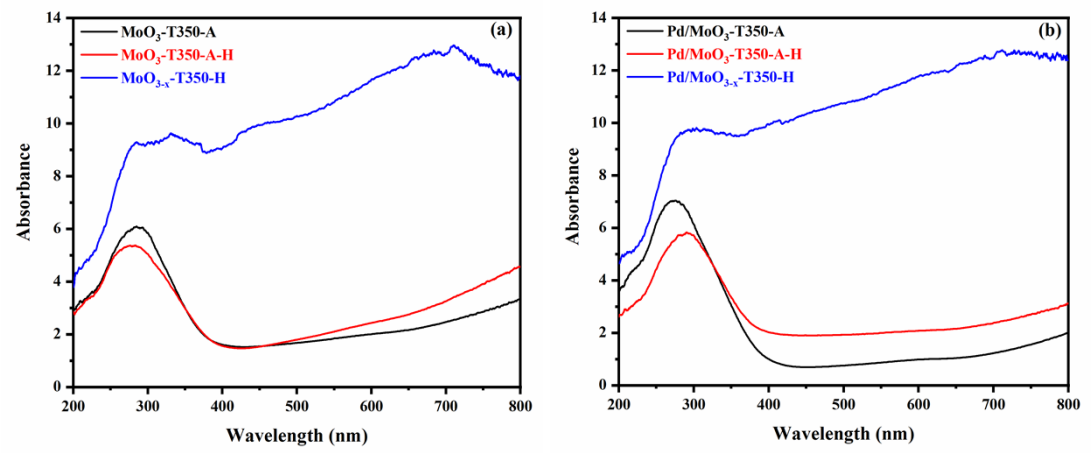

Figure S1. UV-visible absorption spectra of MoO_3 supports (a) and corresponding Pd/MoO_3 catalysts (b).

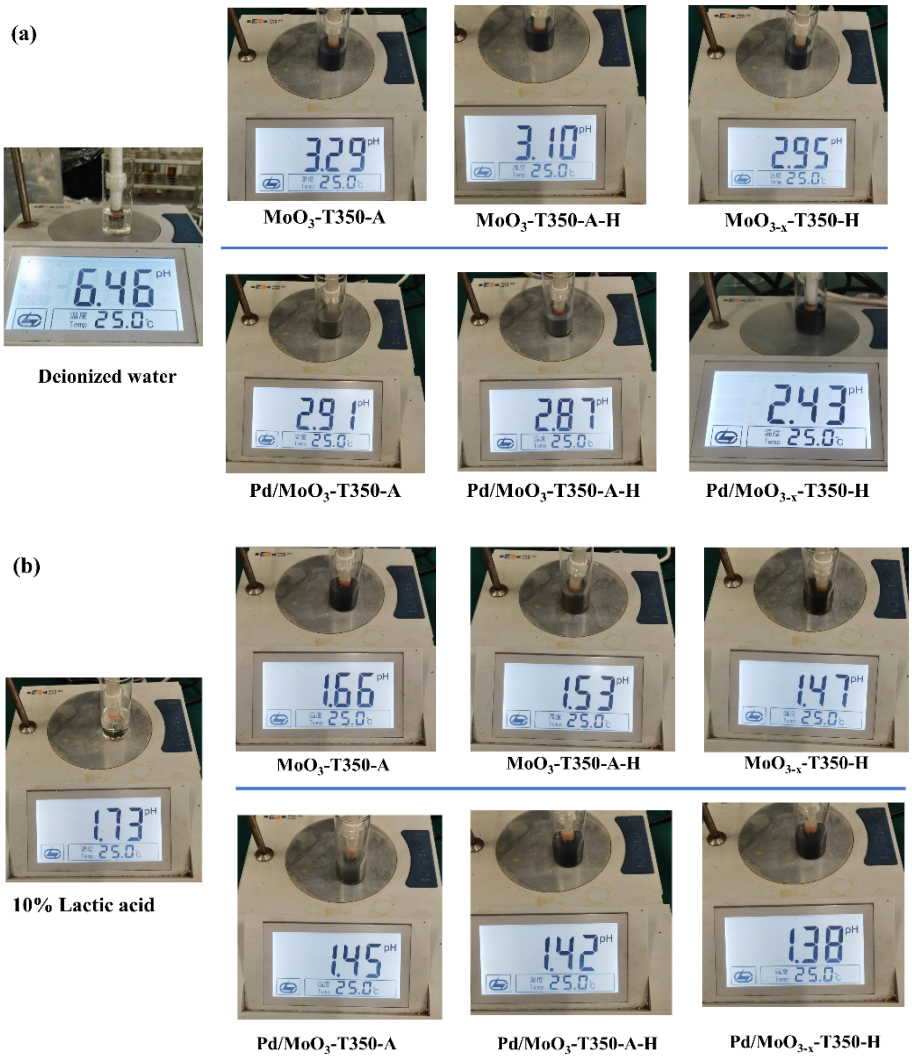

Fig. S2 pH change of pristine supports (a) and their corresponding supported Pd (b) in deionized water and 10 wt% LA aqueous solution.

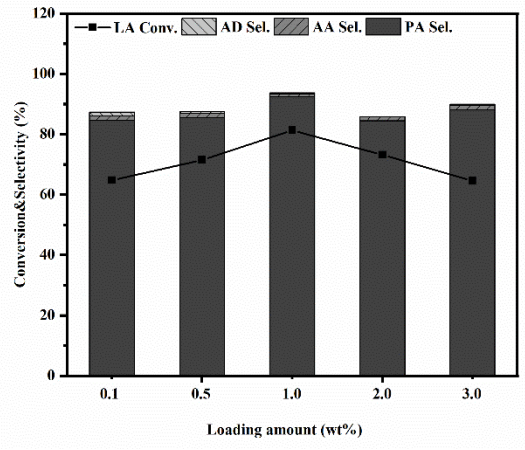

Figure S3. Effect of Pd loading amount on catalytic performance

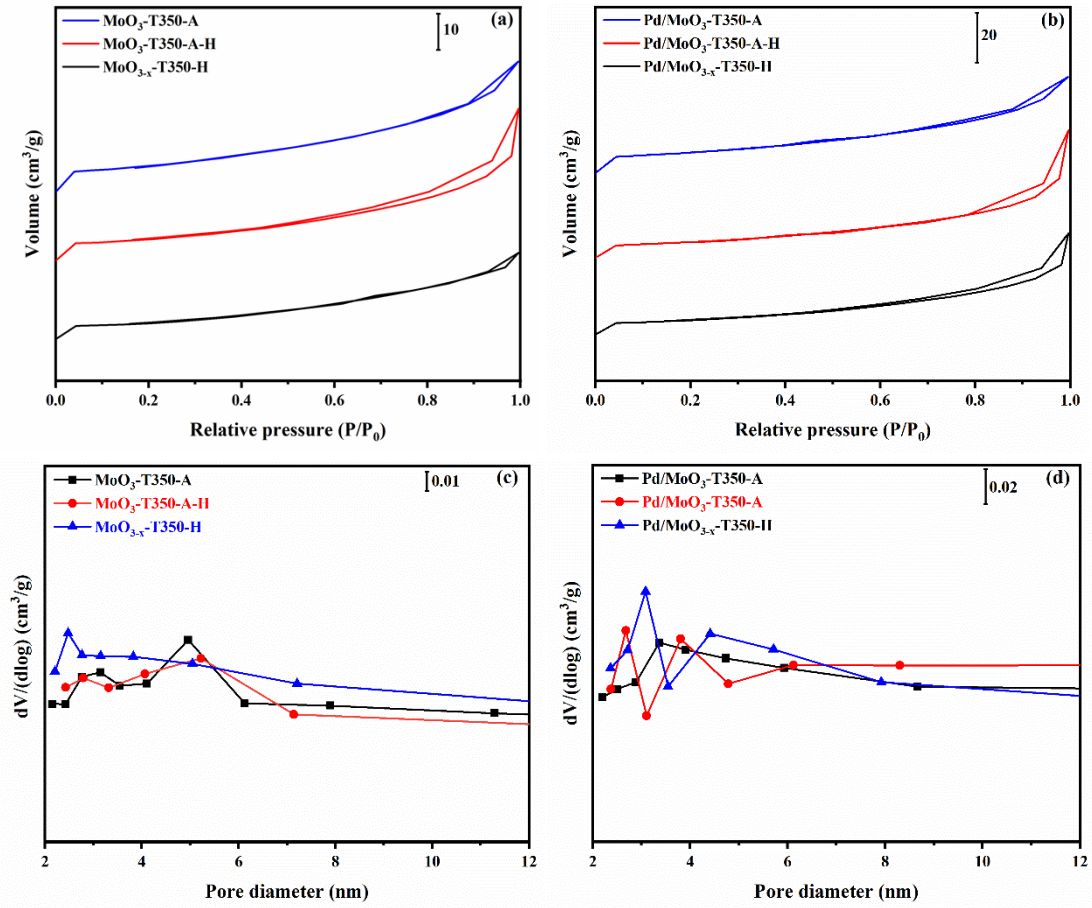

Figure S4. Nitrogen adsorption-desorption isotherm of MoO_3 supports (a) and Pd/MoO_3 catalysts (b); Pore size distribution of MoO_3 supports (c) and Pd/MoO_3 catalysts (d).

Table S1 Energy bands of MoO_3 supports and Pd/MoO_3 catalysts.

Catalyst	E_g (eV)	E_{CB} (eV)	E_{VB} (eV)
MoO_3-T350-A	3.12	-0.01	3.11
MoO_3-T350-A-H	2.97	-0.08	2.89
MoO_{3-x}-T350-H	2.16	-0.18	1.98
Pd/MoO_3-T350-A	2.91	-0.07	2.84
Pd/MoO_3-T350-A-H	2.68	-0.21	2.47
Pd/MoO_{3-x}-T350-H	1.38	-0.3	1.08

Table S2. Comparison of HDO Reactivity in the Conversion of Lactic Acid to Propionic Acid for Pd/MoO_3 catalysts, along with Other HDO Catalysts from the Literature.

Entry	Catalyst	Reaction system	Reaction temp. (ºC)	LA Conv. (%)	PA Sel. (%)	Ref.
1	Pd/MoO_{3-x}-T350-H	heterogeneous	215	81.3	92.4	This work
2	$MoO_2(acac)_2$	homogeneous	270	85.0	52.0	[1]
3	Fe_xO_y	heterogeneous	390	96.7	46.7	[2]
4	Fe_3O_4	heterogeneous	390	93.2	58.4	[3]
5	MoO_2	heterogeneous	390	96.8	62.8	[4]
5	Co-Zn	heterogeneous	250	88.0	66.8	[5]
6	NaI	homogeneous	220	100	99.0	[6]
7	$^{SS}MoS2$	heterogeneous	215	96.8	96.3	[7]

Table S3 Pd Leaching rate in the conversion of lactic acid to propionic acid for Pd/MoO_{3-x} tested by ICP-MS.

Catalyst	Concentration of Pd in reacted solution (mg/L)	Pd leaching rate (%)
Pd/MoO_{3-x}	0.58	0.26

Catalysts,0.5g; LA feedstock: 20 g, 10 wt%, H_2 initial pressure, 3.0 MPa; Reaction temperature, 215°C; reaction time, 12 h.

Table S4 Effect of the amount of 1,1- Diphenylethylene on the catalytic activity of HDO reactivity in the conversion of lactic acid to propionic acid over Pd/MoO_{3-x}.

1,1-Diphenylethylene : LA (mol)	Conv. of LA (%)	Sel. of PA (%)
1:1	78.3	88.9
2:1	79.7	88.2

Catalyst, 0.5 g; LA feedstock, 20 g (5 wt% LA); H_2 initial pressure, 3.0 MPa; Reaction temperature, 215°C; reaction time, 12 h.

References

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