

Supporting Information (SI)

The synergic effect of h -MoO₃, α -MoO₃, and β -MoO₃ phase mixture as a solid catalyst to obtain methyl oleate

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1. Complementary Rietveld Refinement Results

The complementary study of crystallographic information of samples MoO₃_2.5, MoO₃_5, MoO₃_7.5, and MoO₃_10, is performed out by structural Rietveld refinement, in focus, the lattice parameters, unit cell volume, crystallite size and phase composition.

Table S1: Rietveld refinement results obtained for samples MoO₃_2.5, MoO₃_5, MoO₃_7.5, and MoO₃_10.

Parameters	Samples				ICSD	ICSD	ICSD
	MoO ₃ _2.5	MoO ₃ _5	MoO ₃ _7.5	MoO ₃ _10	87962	76651	80577
h-MoO₃							
<i>a</i> (Å)	10.575(3)	10.574(3)	10.578(1)	10.468(7)	10.576(1)		
<i>b</i> (Å)	10.575(3)	10.574(3)	10.578(1)	10.468(7)	10.576(1)		
<i>c</i> (Å)	3.725(7)	3.725(7)	3.725(7)	3.708(2)	3.728(1)		
<i>V</i> (Å ³)	360.85(02)	360.78(2)	361.03(9)	351.94(7)	361.12(12)		
\bar{D}_{hkl} (nm)	46	55	56	77			
X _r (%)	100	97.96	95.71	9.38			
α-MoO₃							
<i>a</i> (Å)		13.855(9)	13.867(3)	13.758(5)		13.8550	
<i>b</i> (Å)		3.696(5)	3.6949(4)	3.672(7)		3.7010	
<i>c</i> (Å)		3.959(7)	3.957(7)	3.940(1)		3.9620	
<i>V</i> (Å ³)		202.81(1)	202.78(1)	199.09(9)		203.16	
\bar{D}_{hkl} (nm)		22	21	20			
X _r (%)		2.04	4.29	73.78			
β-MoO₃							
<i>a</i> (Å)				3.936(5)			3.954(1)
<i>b</i> (Å)				3.670(2)			3.687(2)
<i>c</i> (Å)				7.078(3)			7.095(4)
<i>V</i> (Å ³)				99.38(9)			100.47(8)
\bar{D}_{hkl} (nm)				120			
X _r (%)				16.84			

Legend: *V* = Unit cell volume; \bar{D}_{hkl} = crystallite size and X_r = phase composition.

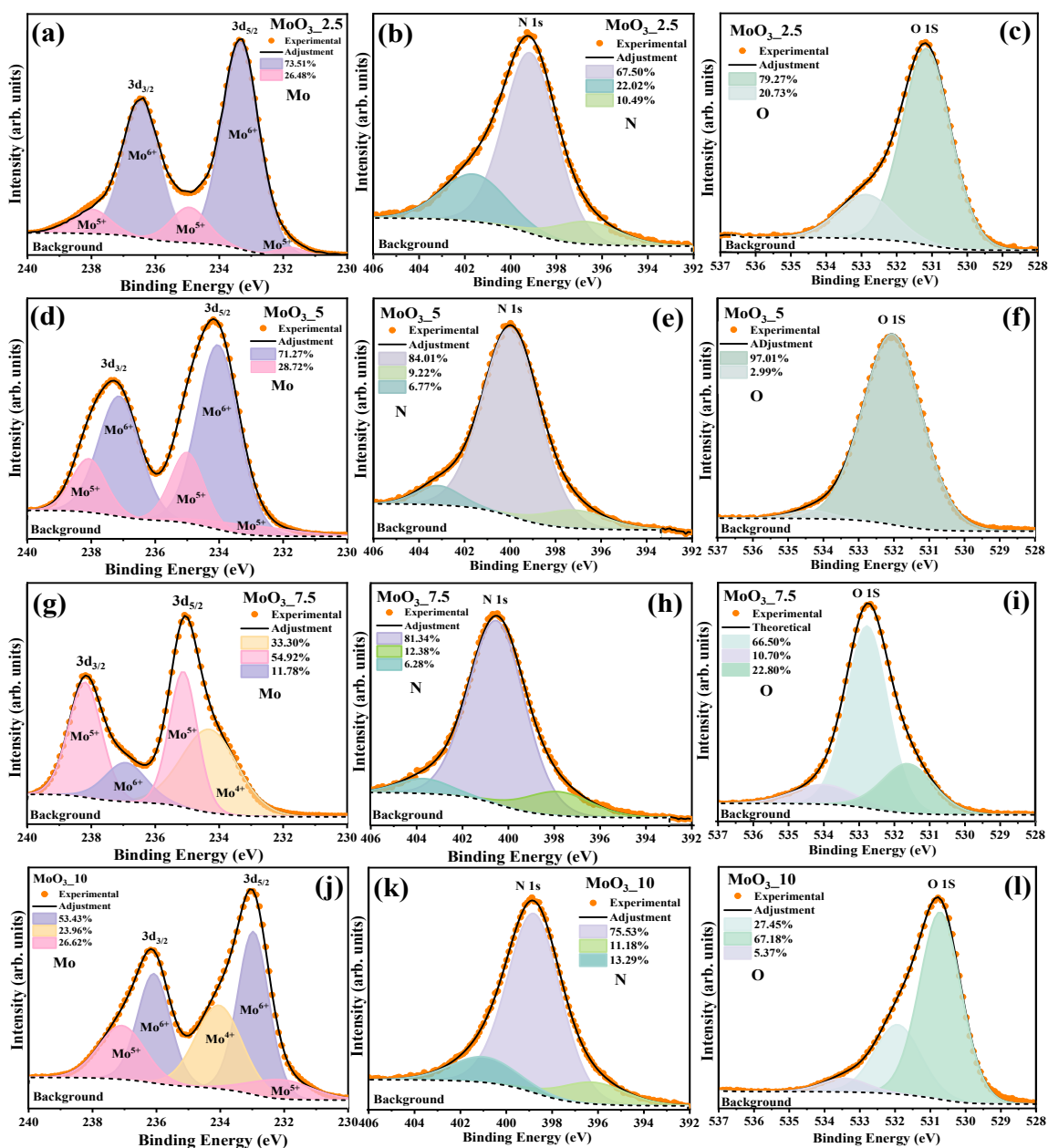


Figure S1: Deconvoluted high resolution Mo 3d_{3/2} and 3d_{5/2}, O 1s and N 1s XPs spectrum of Rietveld refinement results obtained for samples (a-c) MoO₃_2.5, (d-f) MoO₃_5, (g-i) MoO₃_7.5, and (j-l) MoO₃_10.