

Supplementary Information

Catalytic conversion of sucrose to 1,2-propanediol over alumina supported Ni-Mo bimetallic catalyst

Sreejith Sreekantan^{a,b}, Arun Arunima Kiralja^{a,b}, Banu Marimuthu,^{*ab}

^aCatalysis and Inorganic Chemistry Division,
CSIR-National Chemical Laboratory, Dr.Homi Bhabha Road, Pune-411008, India

^bAcademy of Scientific and Innovative Research, Ghaziabad, Uttar Pradesh- 201 002, India

KEYWORDS : Biomass conversion, Sugar hydrogenolysis, propylene glycol, Retro-aldol condensation, Renewable resources, Sustainability.

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1. The reaction data of different Ni-Mo supported over γ -Al₂O₃ catalyst on sucrose substrate

Table S1 : The optimisation of different Ni-Mo bimetallic combinations over γ -Al₂O₃ support at 220°C, 40 bar H₂, 4.5 h, 2 wt% Sucrose

Entry No	Metal Loading (%)		Product Selectivity (%)							
	Ni	Mo	1,2-PDO	1,3-PDO	EG	1,2-BDO	2-PrOH	1-PrOH	Lactic Acid	EG+PDO+BDO
1	6	20	70.1	1.0	4.1	15.3	1.0	1.7	2.2	90.5
2	10	20	67.1	0.4	7.2	11.4	2.9	1.8	2.4	86.1
3	8	20	72.2	1.1	4.6	11.7	2.2	2.0	3.1	89.6
4	8	15	61.2	Trace	2.9	12.0	8.2	Trace	7.0	76.1
5	8	25	69.4	0.8	5.5	12.6	1.4	1.3	2.3	88.3
6	8	0	30.4	0.6	6.3	3.1	3.6	ND	20.0	40.4
7	0	20	15.7	1.2	14.0	2.1	4.2	ND	32.2	33.0
8	0	0	19.9	1.3	14.6	2.2	3.7	ND	29.8	38.0

2. The optimisation of the reaction conditions using 8%Ni-20%Mo/ γ - Al₂O₃ catalysts

Table S2: The optimisation of the reaction conditions for active catalyst (8%Ni-20%Mo/ γ - Al₂O₃) on sucrose substrate

Entry No	Reaction Conditions					Product Selectivity (%)					
	T (°C)	P (bar)	Sucrose: Catalyst Ratio	Sucrose Concentration (wt%)	Time (h)	1,2-PD	1,3-PD	EG	1,2-BDO	Lactic Acid	PDO+ EG+BDO
1	220	40	1:0.35	2	4.5	72.2	1.1	4.6	11.7	3.1	89.6
2	200	40	1:0.35	2	4.5	71.6	Trace	4.6	11.9	3.2	88.1
3	180	40	1:0.35	2	4.5	73.7	2.6	2.5	12.2	1.8	91.0
4	160	40	1:0.35	2	4.5	46.0	6.0	1.9	8.7	Trace	62.6
5	180	50	1:0.35	2	4.5	70.0	3.2	5.8	10.8	2.6	89.8
6	180	30	1:0.35	2	4.5	67.6	3.9	4.0	11.6	3.2	87.1
7	180	40	1:0.5	2	4.5	70.6	2.6	4.6	13.1	2.0	90.9
8	180	40	1:0.20	2	4.5	53.1	5.6	3.9	10.5	6.6	73.1
9	180	40	1:0.35	2	2.5	70.8	4.1	2.5	12.9	2.4	90.3
10	180	40	1:0.35	2	6.5	71.7	1.8	3.1	13.6	2.5	90.2
11	180	40	1:0.35	5	4.5	73.5	3.7	1.4	14.3	3.2	92.9

3. The reusability study of the catalyst 8%Ni-20%Mo/ γ - Al₂O₃ catalyst

Table S3: The reusability of the 8%Ni-20%Mo/ γ - Al₂O₃ over 2wt% sucrose at 180°C, 40bar H₂, 4.5 h run time

# of Run	Product Selectivity (%)					
	1,2-PD	1,3-PD	EG	1,2-BDO	Lactic Acid	PDO+ EG+BDO
Run 1	73.7	2.6	2.5	12.3	1.8	91.1
Run 2	73.2	2.6	3.8	12.8	1.6	92.4
Run 3	70.0	3.0	4.0	10.8	3.4	87.8
Run 4	61.8	1.7	4.3	11.6	6.6	79.4

4. The reusability study of 8%Ni-20%Mo/ γ - Al₂O₃ at lower conversion

Table S4: The reusability of the 8%Ni-20%Mo/ γ - Al₂O₃ over 2wt% sucrose at 160°C, 40bar H₂, 1 h run time

# of Run	Conversion	Product Selectivity (%)						
		1,2-PD	1,3-PD	EG	1,2-BDO	Lactic Acid	1-PrOH	PDO+ EG + BDO
Run 1	54.7	69.0	3.3	1.5	10.1	2.8	2.1	83.9
Run 2	54.4	71.3	2.6	1.2	10.3	0.3	2.6	85.4
Run 3	57.7	69.9	3.1	1.2	9.7	0.9	2.3	83.9

5. The XRD data of fresh and spent catalysts

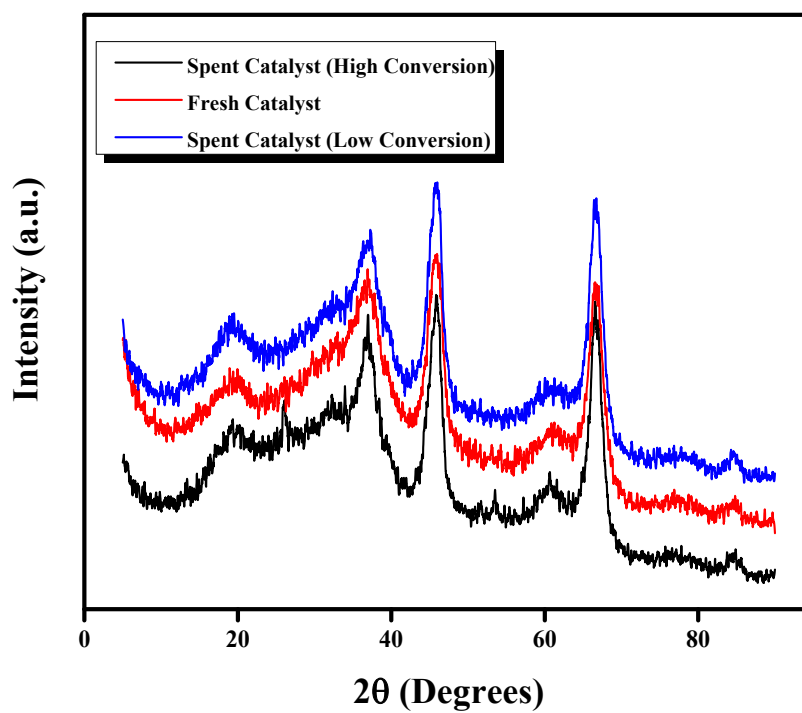


Figure S1: The XRD patterns of the fresh and spent catalyst at low conversion and high conversion

6. The morphology study of used and spent catalyst

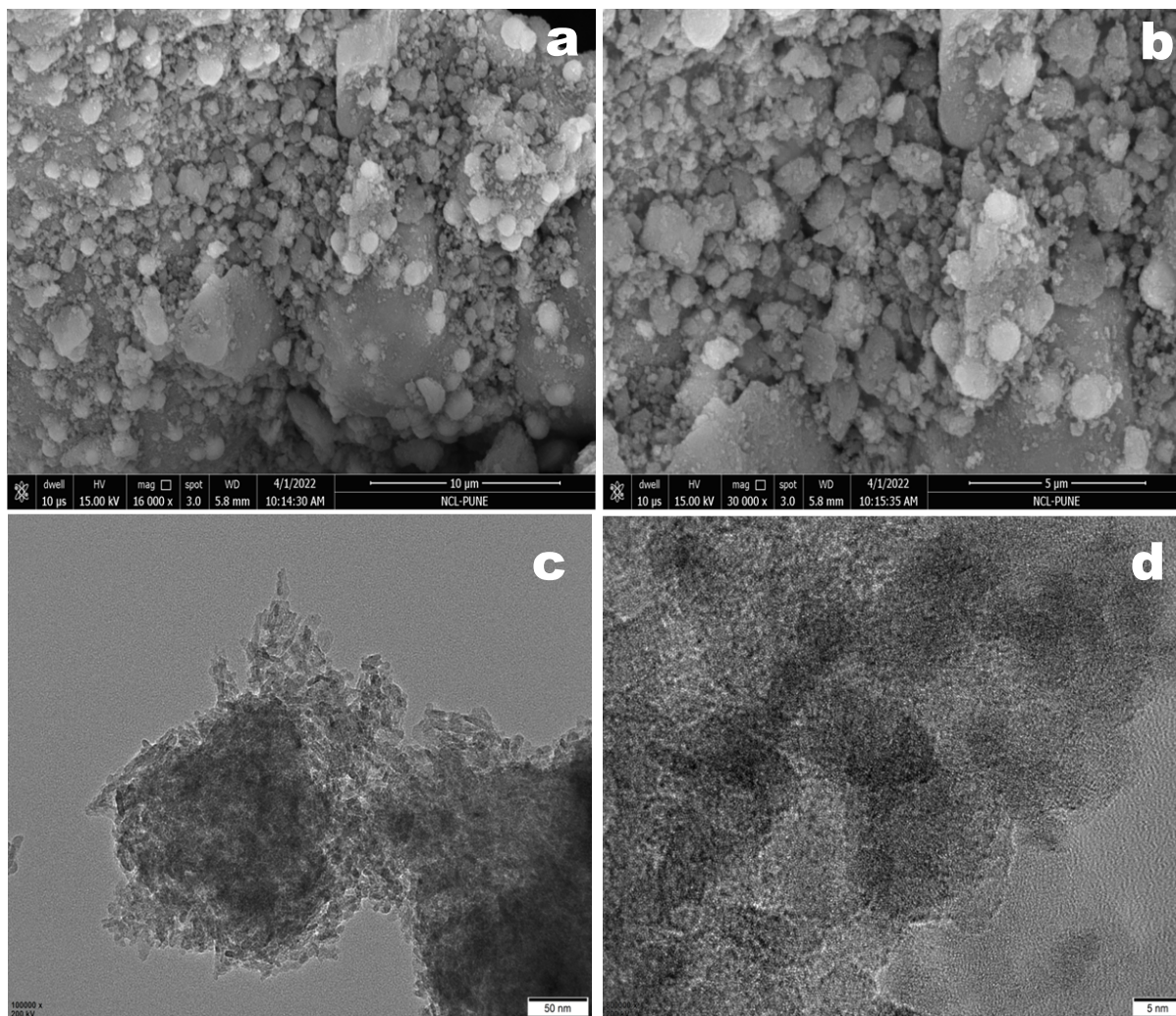


Figure S2: The morphology of the spent catalyst after 4 runs (a & b) FE-SEM (c & d) HR-TEM

7. The pyridine IR of various Ni-Mo/ γ -Al₂O₃ supported catalysts.

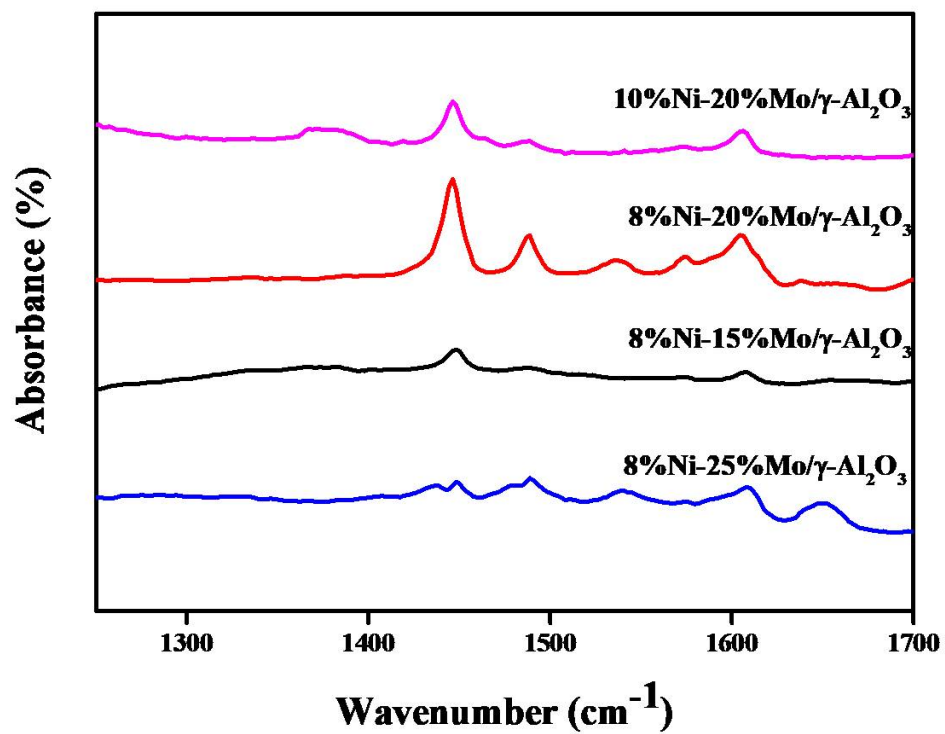


Figure S3 : The py-IR spectra of various γ -Al₂O₃ supported catalysts

8. The deconvoluted XPS spectrum of Ni-2p and Mo-3d various Ni-Mo/ γ -Al₂O₃ catalysts.

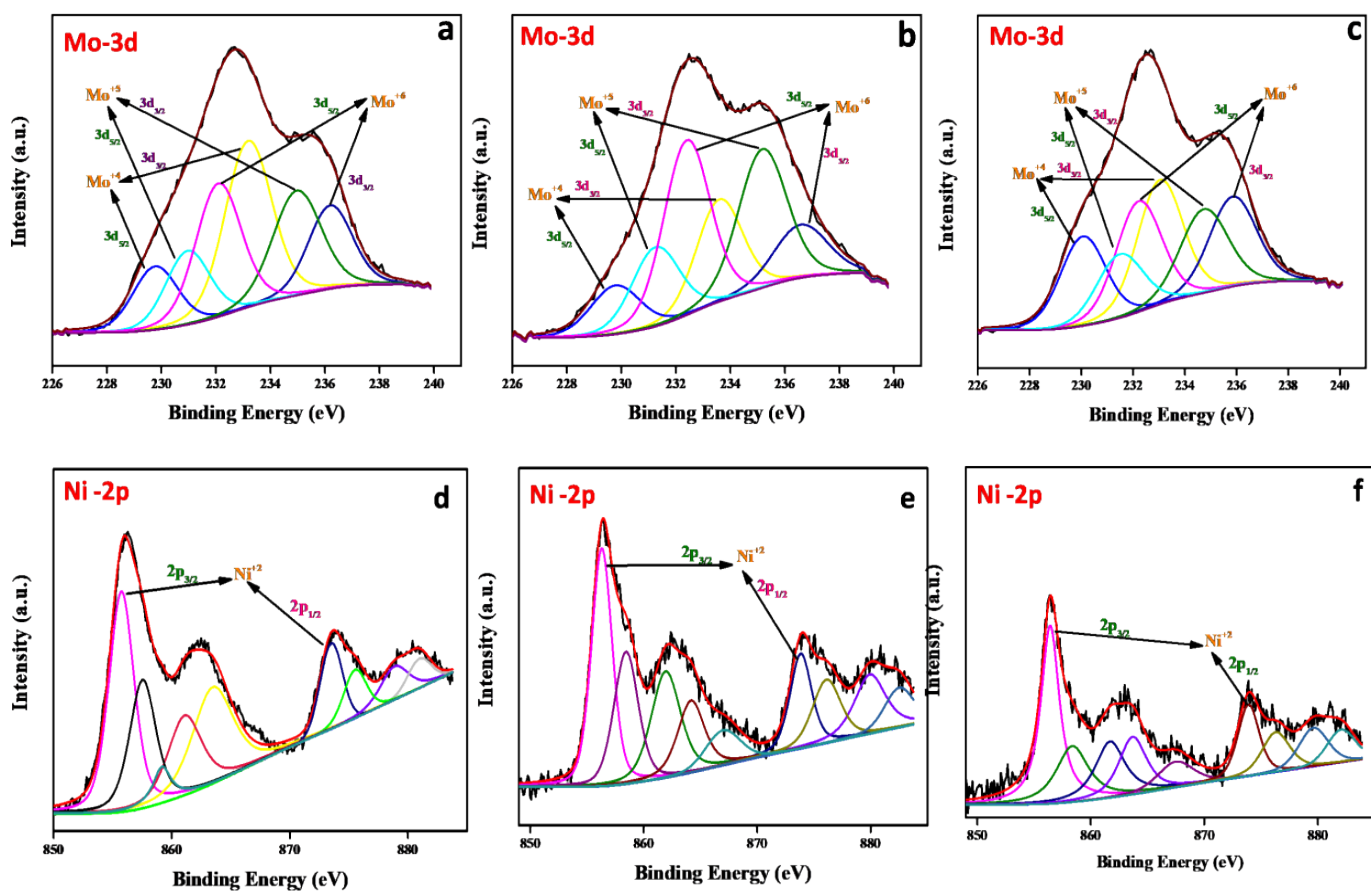


Figure S4 : The deconvoluted XPS of (a) Mo-3d of 20%Mo/ γ -Al₂O₃ (b&e) Mo-3d & Ni-2p of 8%Ni-15%Mo/ γ -Al₂O₃ (c &f) Mo 3d & Ni 2p of 8%Ni - 25%Mo/ γ -Al₂O₃ (d) Ni-2p of 8%Ni/ γ -Al₂O₃

9. The HPLC chromatogram of the activity study of the catalyst 8%Ni-20%Mo/ γ - Al₂O₃ at optimized reaction condition

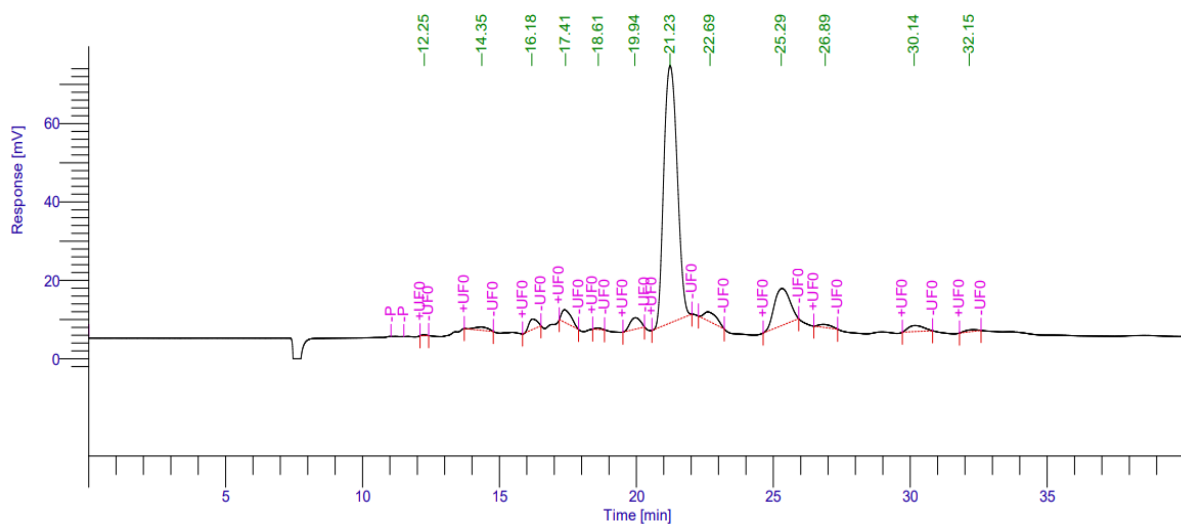


Figure S5: The HPLC chromatogram of the reaction of 8% Ni-20%Mo/ γ - Al₂O₃ over 2wt% sucrose at 180°C, 40 bar H₂, 4.5 h at 1:0.3 sucrose: catalyst ratio

Retention Time	Compound
21.23	1,2- Propanediol
22.89	1,3-Propanediol
19.94	1,2-Ethandiol
25.29	1,2-Butanediol
16.18	Lactic acid
32.15	1-Propanol
17.41	Glycerol

10. The Calibration curve for the 1,2-propanediol

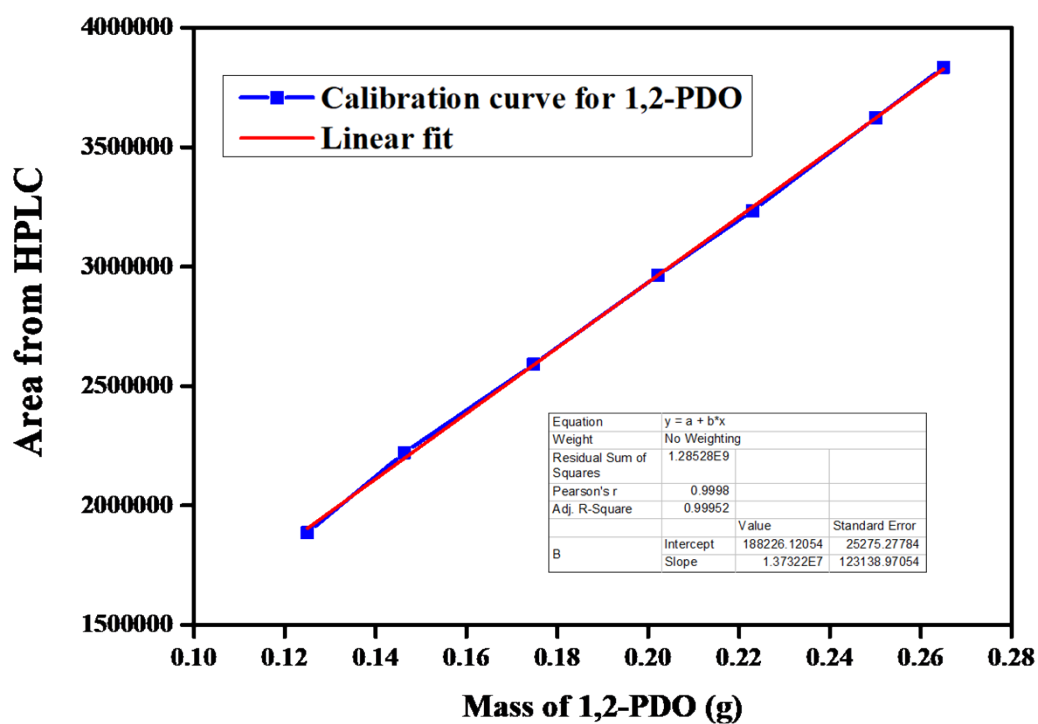


Figure S6: The calibration curve for 1,2-PDO