

Supporting Information

Role of Lattice Strain in Bifunctional Catalyst for Tandem Furfural Hydrogenation-Esterification

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Table S1: Chemicals

Chemical	Purity (%)	Company/Source
Rice husk	100	Penang, Malaysia
Sodium hydroxide, NaOH	≥97	Merck Millipore
Nitric acid, HNO ₃	65 w/w	Riendemann Schmidt Chemical
Copper (II) nitrate Penta hemihydrate, Cu (NO ₃) ₂ .5H ₂ O	≥99	Riedel-de Haën
Nickel (II) nitrate hexahydrate, Ni (NO ₃) ₂ .6H ₂ O	≥99	Sigma Aldrich
Palladium (II) nitrate dehydrate, Pd (NO ₃) ₂ .2H ₂ O	≥99	Sigma Aldrich
Aluminium Isopropoxide, AIP	≥98	Sigma Aldrich
Magnesium nitrate, Mg (NO ₃) ₂	≥99	Merck Millipore
Furfural	≥99	Sigma Aldrich
Acetic acid, glacial	≥99	Sigma Aldrich
Ethanol	≥99.8	Sigma Aldrich
Pyridine, anhydrous	≥99.8	Sigma Aldrich

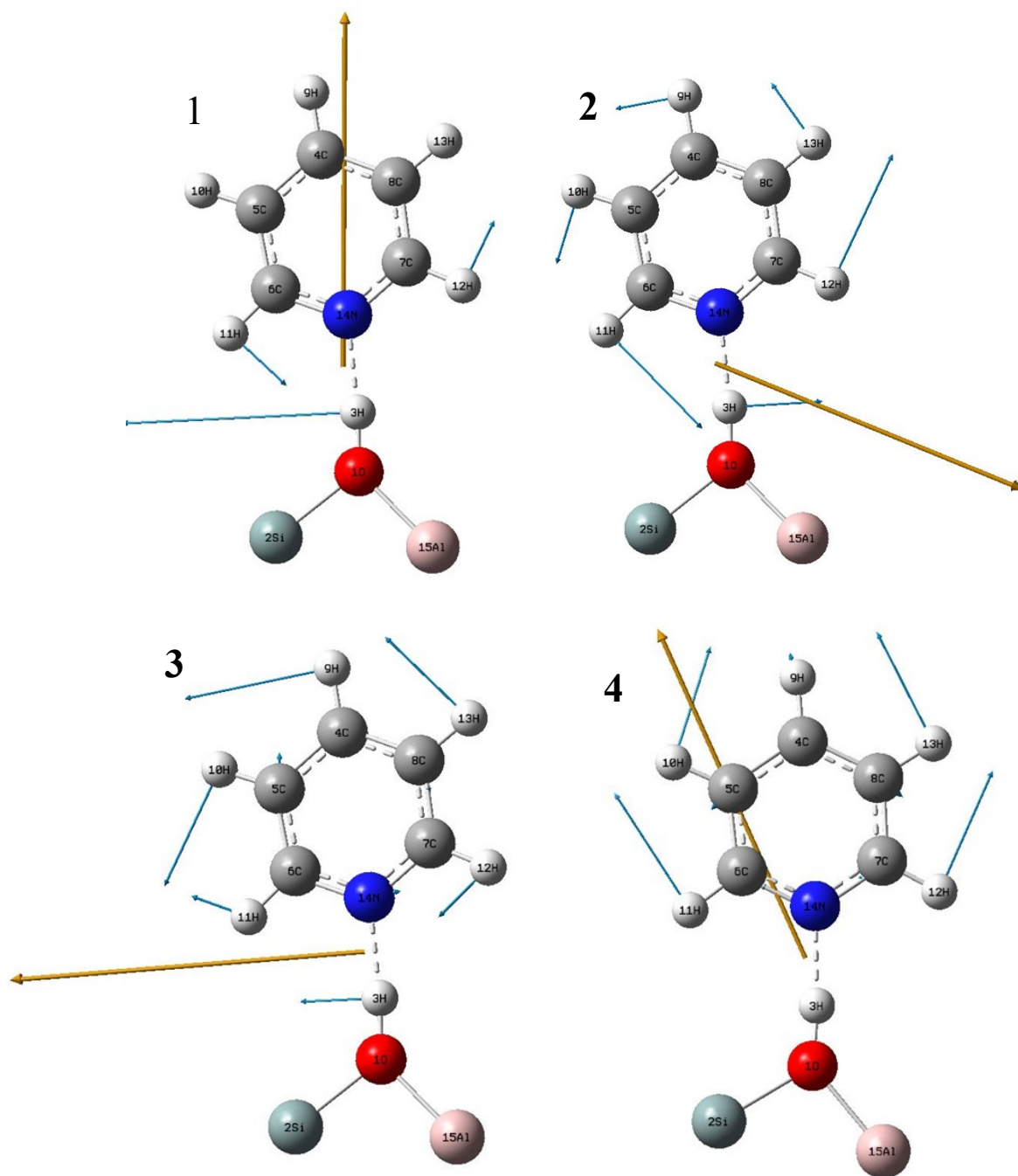


Fig. S1: The dipole moment and dipole derivative of pyridine adsorbed on Brønsted acid sites for single metal-doped ($M = \text{Cu}, \text{Ni}, \text{ and } \text{Pd}$)/ $\text{RHSiO}_2\text{-Al-Mg}$.

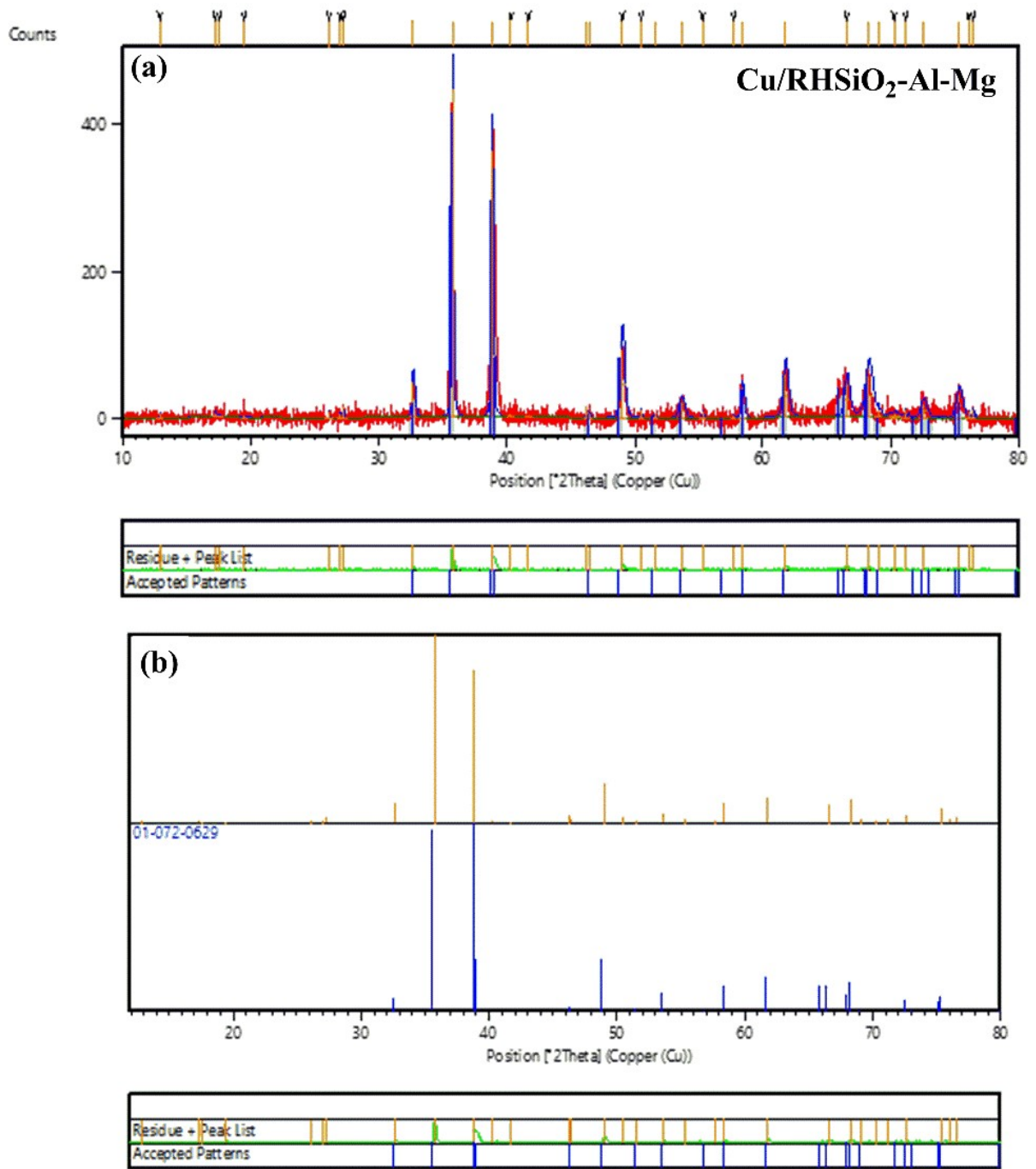


Fig. S2: (a) Peak lists of Cu/RHSiO₂-Al-Mg (b) Experimental-library matches of Cu/RHSiO₂-Al-Mg

Table S2: Crystal parameters of Cu/RHSiO₂-Al-Mg

Reference Code	01-072-0629
Compound Name	Copper oxide
Crystal System	Monoclinic
Space Group	C2/c
Space Group Number	15
A (Å)	4.6837
B (Å)	3.4226
C (Å)	5.1288
Alpha (°)	90.0000
Beta (°)	99.5400
Gamma (°)	90.0000
Calculated Density (g/cm³)	6.51
Volume Of Cell (10⁶ pm³)	81.08
Z	4.00
R_{int}	3.90

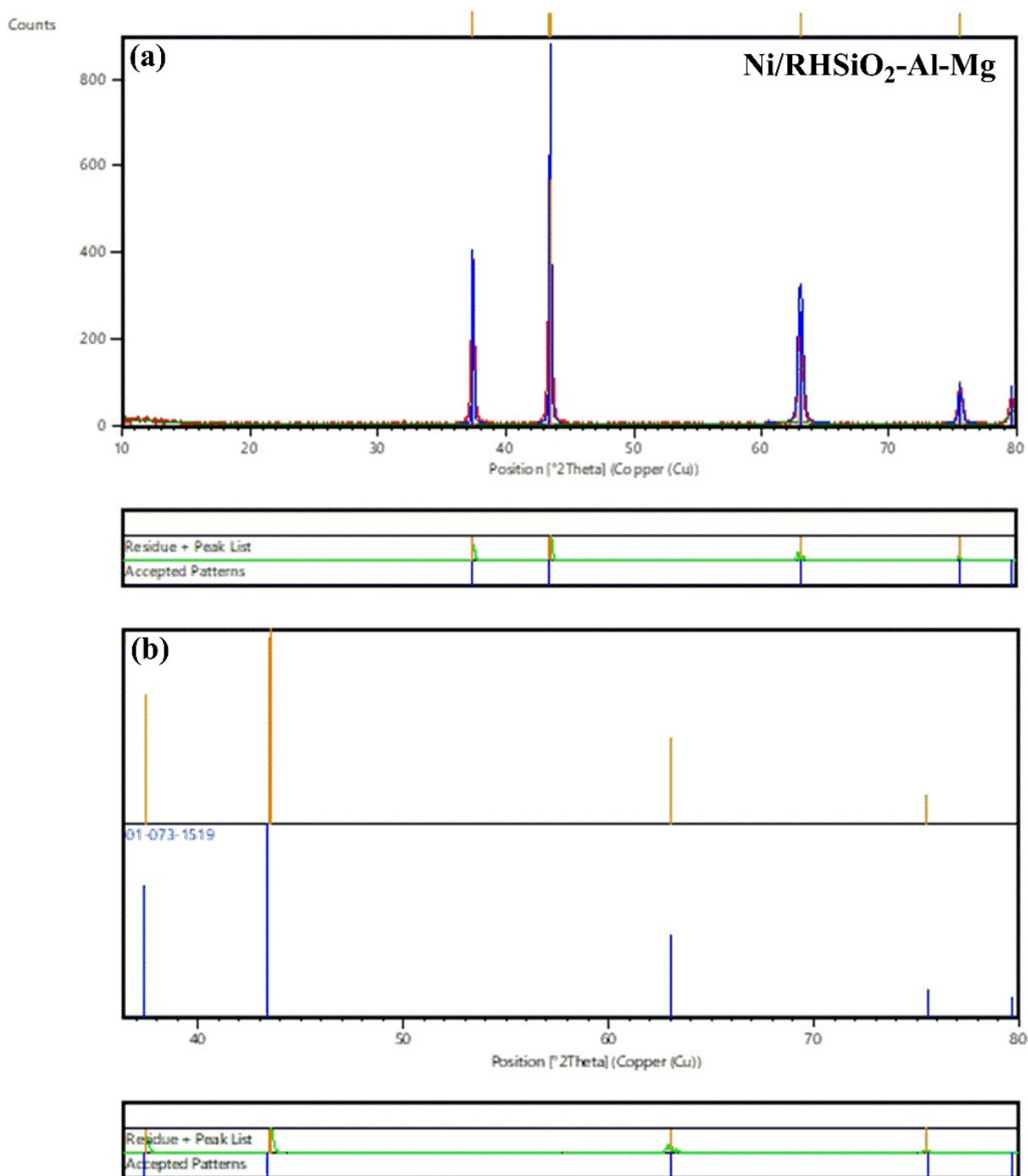


Fig. S3: (a) Peak lists of Ni/RHSiO₂-Al-Mg (b) Experimental-library matches of Ni/RHSiO₂-Al-Mg

Table S3: Crystal parameters of Ni/RHSiO₂-Al-Mg

Reference code	01-073-1519
Compound name	Nickel oxide
Crystal system	Cubic
Space group	Fm-3m
Space group number	225
A (Å)	4.1684
B (Å)	4.1684
C (Å)	4.1684
Alpha (°)	90.0000
Beta (°)	90.0000
Gamma (°)	90.0000
Calculated density (g/cm³)	6.85
Volume of cell (10⁶ pm³)	72.43
Z	4.00
R_{int}	4.74

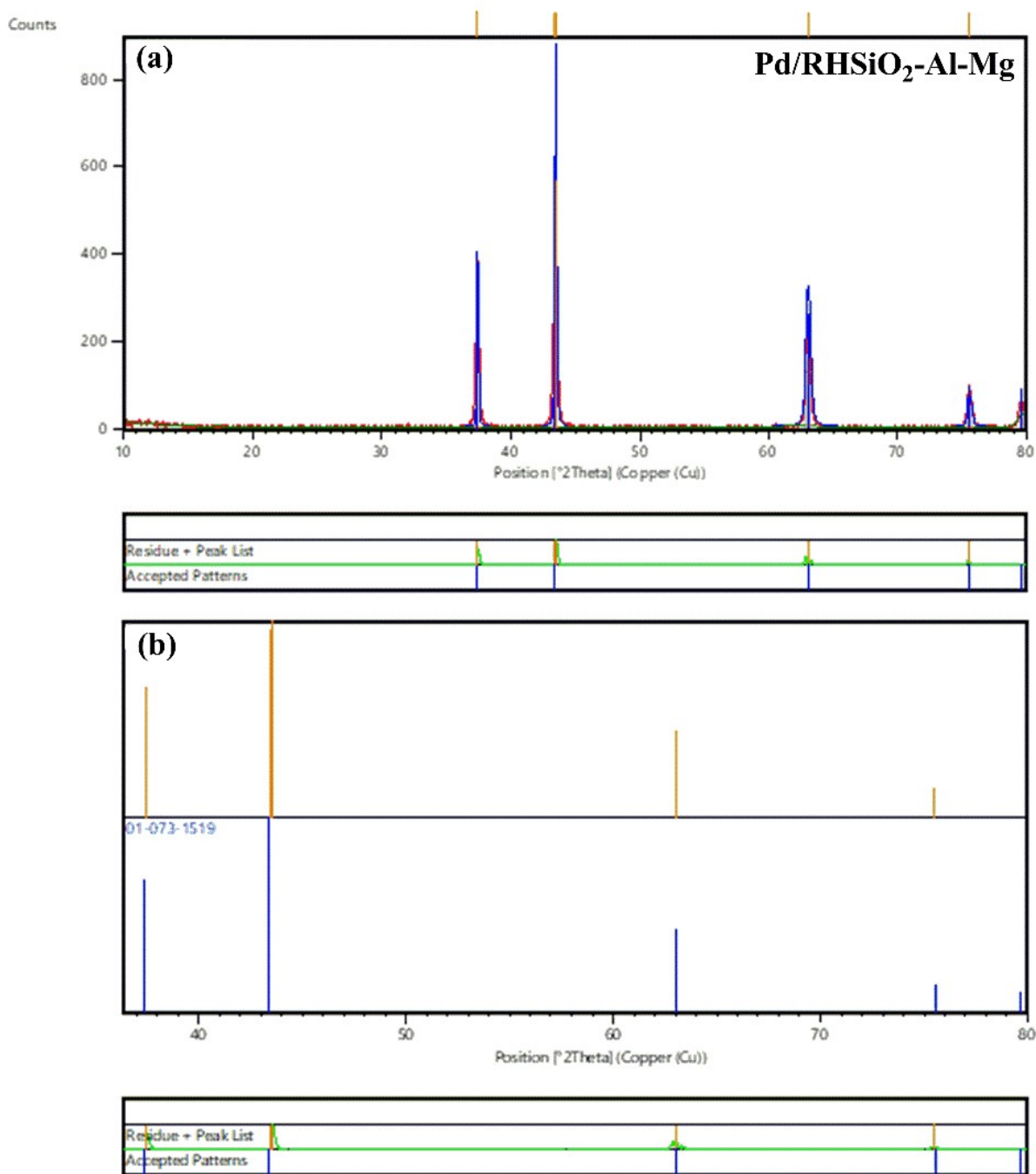
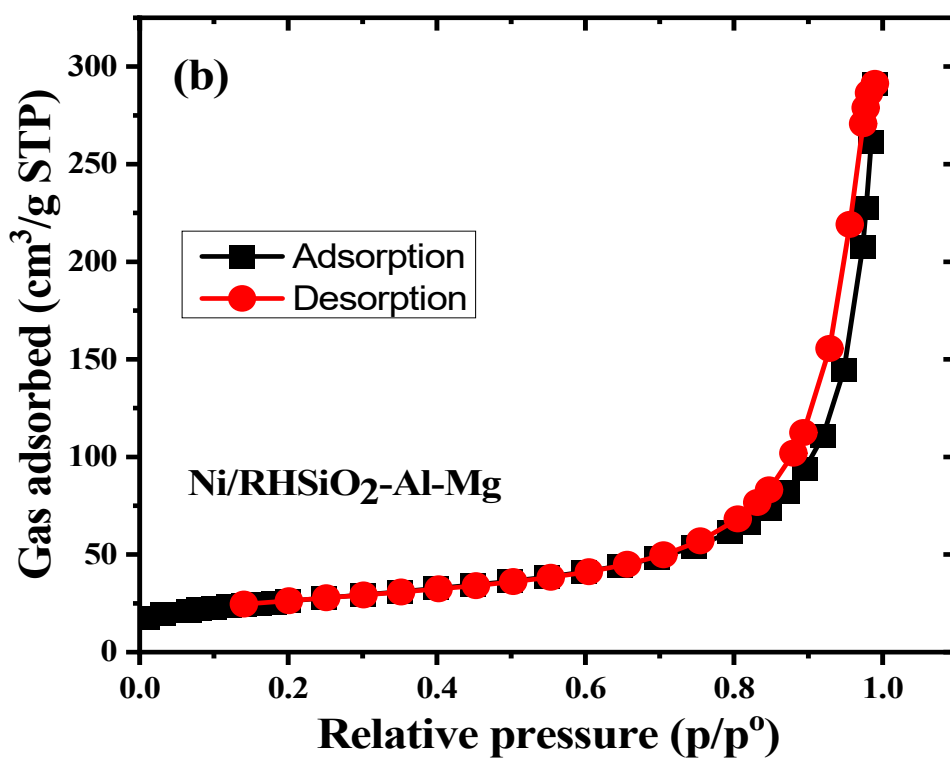
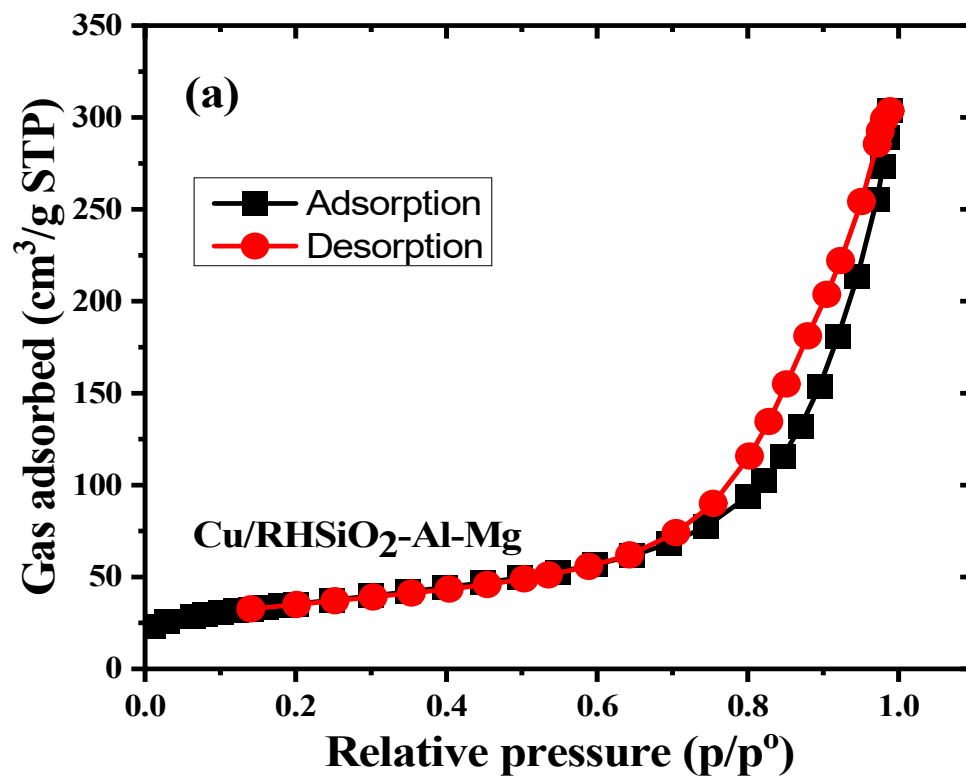


Fig. S4: (a) Peak lists of Pd/RHSiO₂-Al-Mg (b) Experimental-library matches of Pd/RHSiO₂-Al-Mg

Table S4:
parameters of
Mg

Crystal
Pd/RHSiO₂-Al-

Reference code	01-075-0584
Compound name	Palladium Oxide
Crystal system	Tetragonal
Space group	P-4n2
Space group number	118
A (Å)	3.0360
B (Å)	3.0360
C (Å)	5.3270
Alpha (°)	90.0000
Beta (°)	90.0000
Gamma (°)	90.0000
Calculated density (g/cm³)	8.28
Volume of cell (10⁶ pm³)	49.10
Z	2.00
Rir	14.48



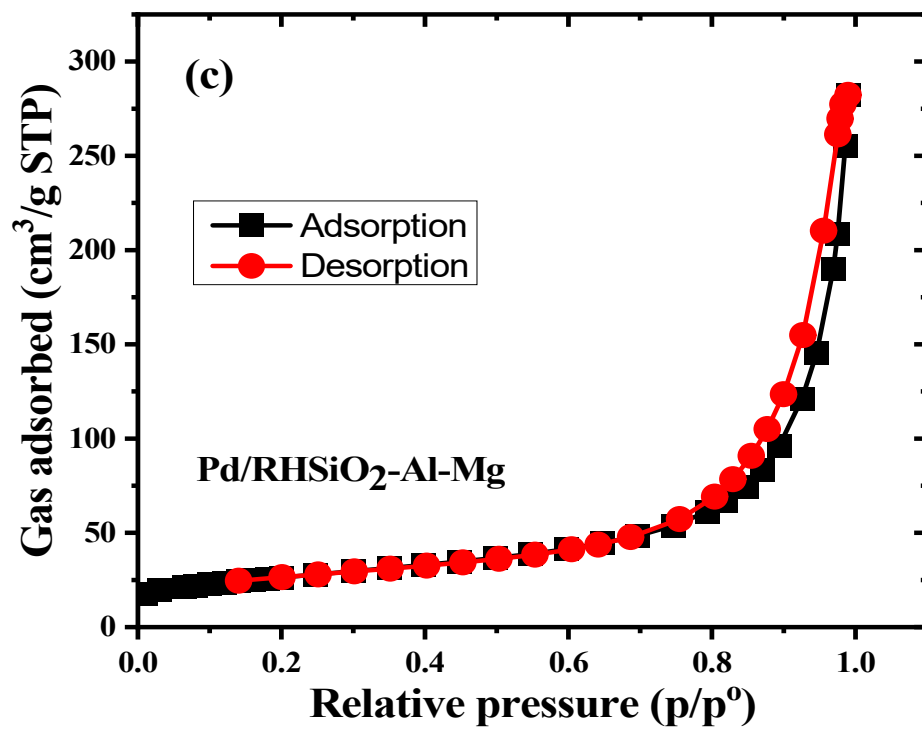


Fig. S5: BET hysteresis loop

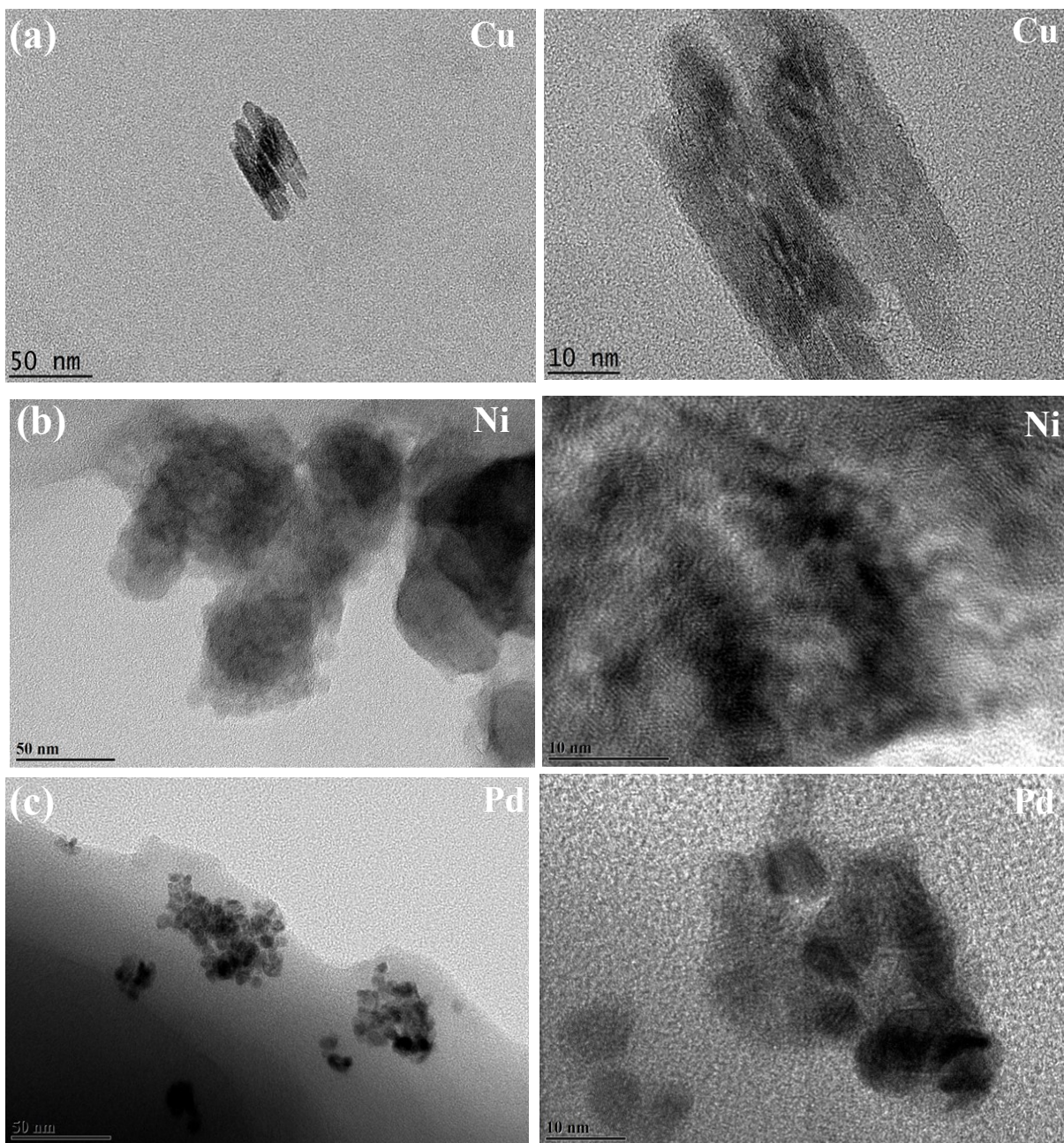


Fig. S6: Reused catalysts HR-TEM