Supplementary file

Hydrogenation of CO_2 to synthetic natural gas (SNG) with 100 % selectivity over a Ni-ZnO-MgO catalyst

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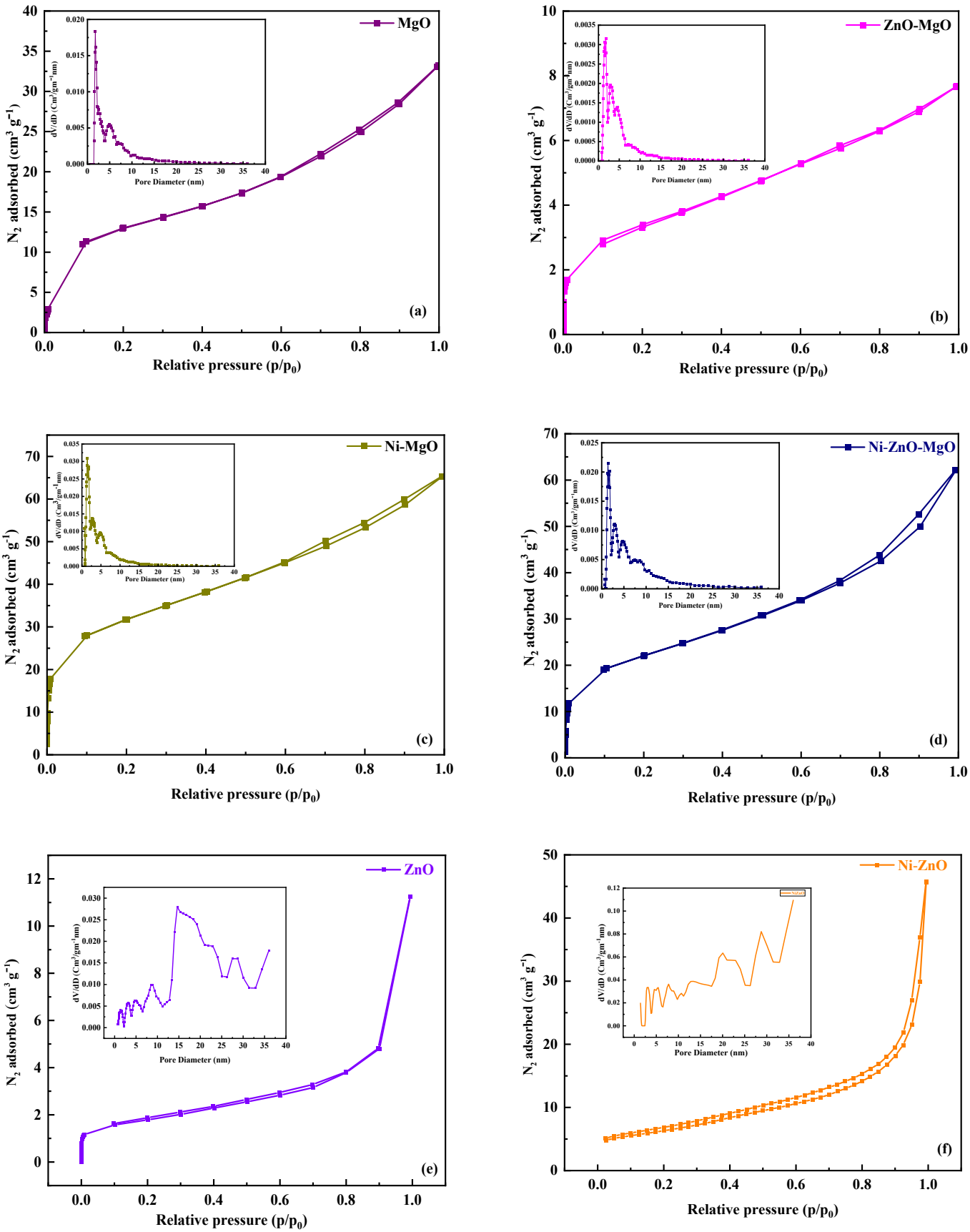

Fig. S1. Nitrogen adsorption-desorption isotherm and pore size distributions of synthesized

catalysts, (a) MgO, (b) ZnO-MgO, (c) Ni-MgO, (d) Ni-ZnO-MgO, (e) ZnO, (f) Ni-ZnO

Table S1

Physicochemical properties of the catalysts

Catalyst	Surface area (m^2/g)	Average pore diameter (nm)	Total pore volume (cc/g)	Crystalite size (nm)			Ni metal dispersion (%)	Ni metal surface area (m^2/g_{cat})
				MgO	NiO	ZnO		
MgO	49.60	11.07	0.08	16.90	-	-	-	-
NiO-MgO	42.10	12.60	0.13	14.10	21.40		1.22	4.06
ZnO-MgO	11.50	7.30	0.03	21.30	-	13.80		
Ni-ZnO-MgO	33.80	16.40	0.14	21.30	21.40	20.90	2.54	8.12
ZnO	8.00	11.40	0.02	-	-	13.80	-	-
NiO-ZnO	22.20	10.50	0.06	-	14.30	13.80	0.69	3.25

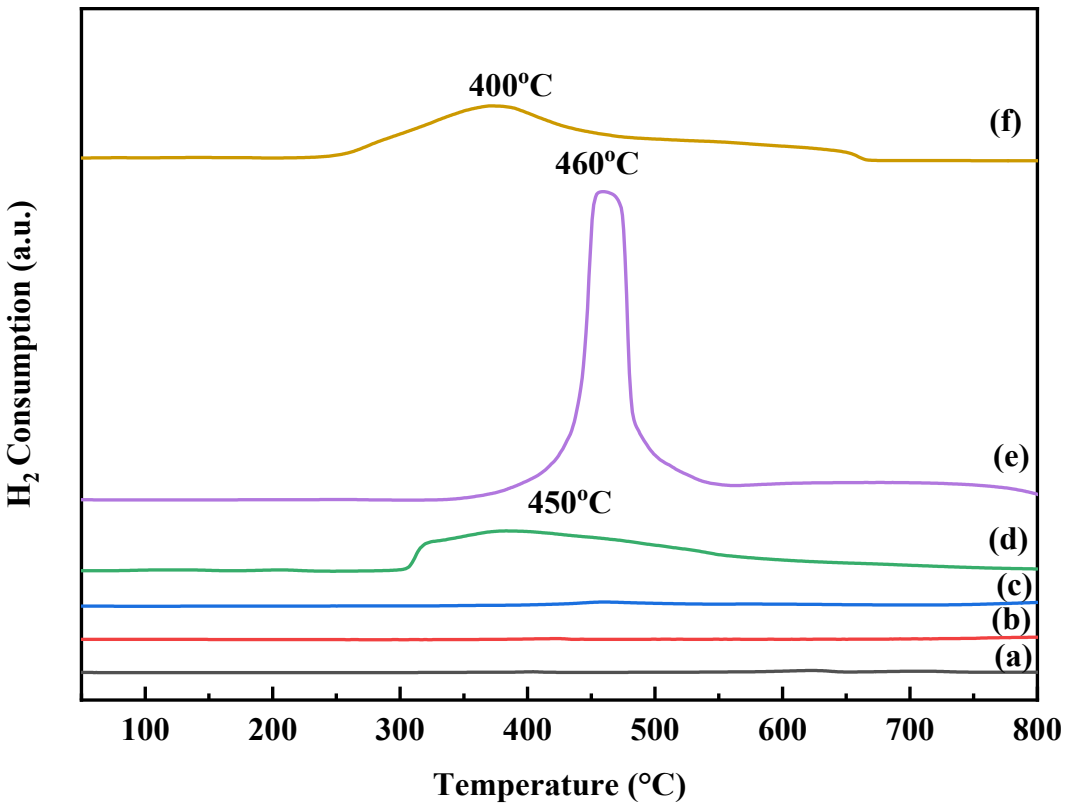

Fig. S2. TPR profiles of catalyst, (a) MgO, (b) ZnO, (c) ZnO-MgO, (d) NiO-MgO, (e) NiO-ZnO, (f) Ni-ZnO-MgO.

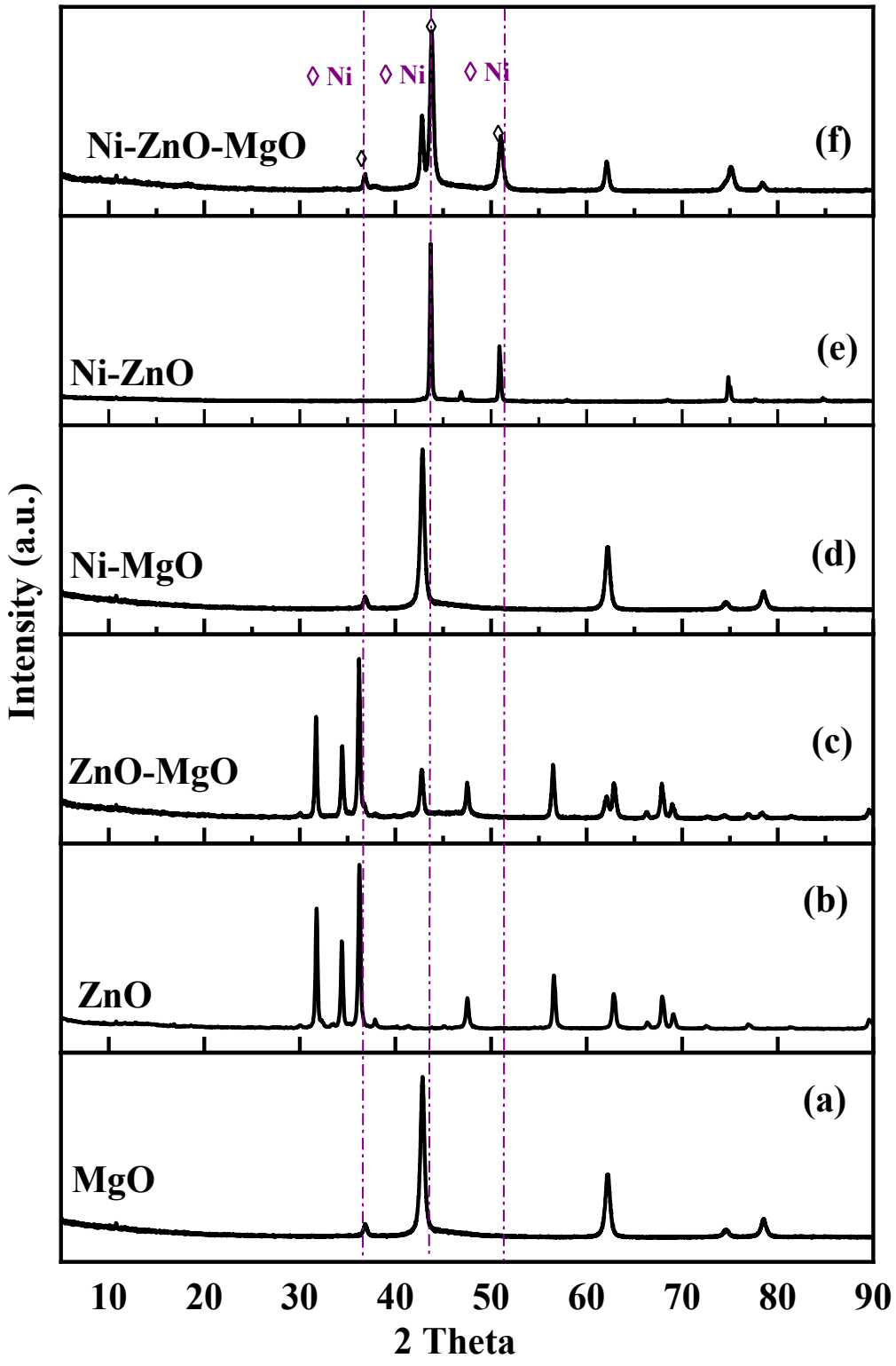

Fig. S3 . Diffraction patterns of reduced catalysts (a) MgO, (b) ZnO, (c) ZnO-MgO, (d) Ni-MgO, (e) Ni-ZnO, and (f) Ni-ZnO-MgO

Used catalyst characterization

S.4 TGA

The TGA patterns of the fresh and used catalyst is compared in Fig. S5. TGA was performd in the presence of air to evaluate the carbon deposition if any. For both the catalyst weight loss below 200°C was observed due to the loss of moisture. Further, in between 200-380°C the weight gain was observed due to the catalyst reoxidation. At higher temperature (>380°C), weight loss was observed for the spent catalyst due to the oxidation of the carbon deposited during the reaction. Based on the TGA data the carbon deposition rate as calculated and it was ~0.016 $g_c.g^{-1}_{cat.}.h^{-1}$. [1, 2]. The weight loss of the fresh catalyst was negligible after 400°C.

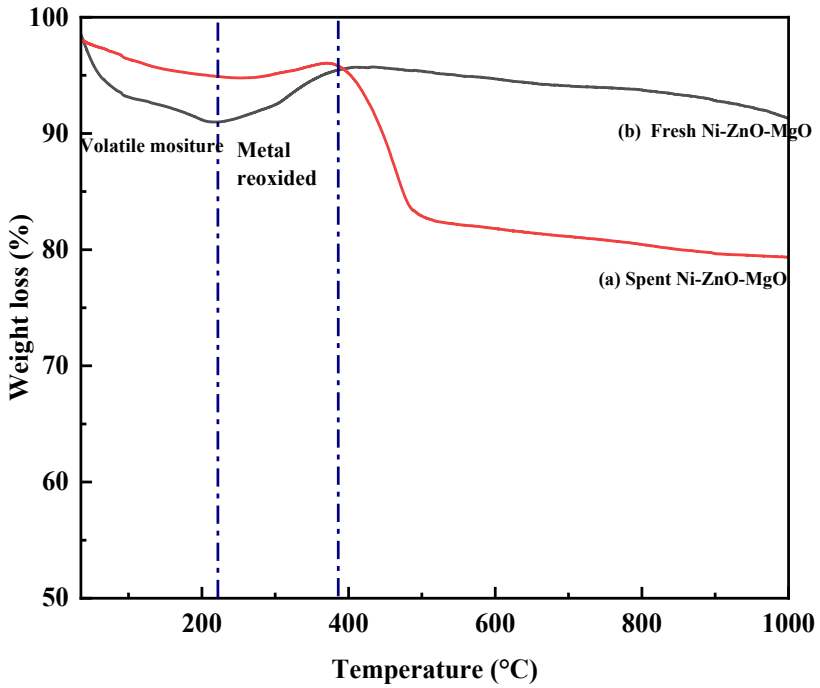

Fig. S4. TGA patterns of fresh and spent Ni-ZnO-MgO catalyst.

S.5 EDX

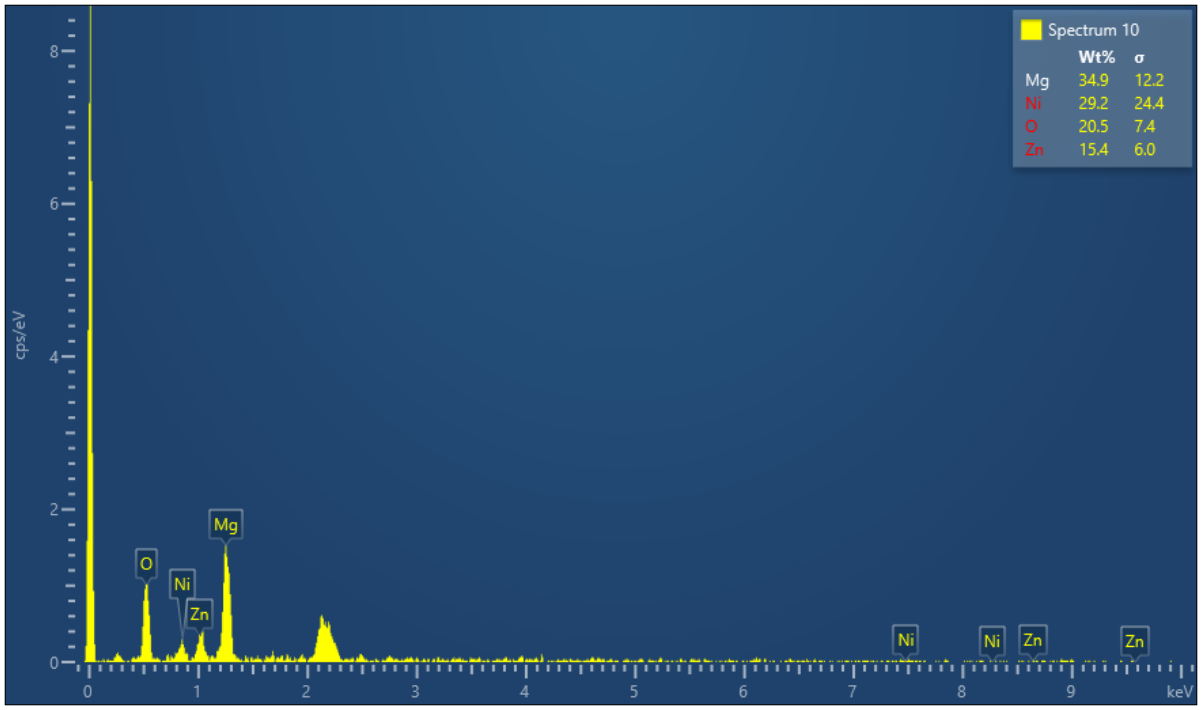

Fig. S5. EDX analysis of Ni-ZnO-MgO catalyst.

Table S2

Elemental composition of the catalyst

Catalyst	Theoretical weight (%)	weight (%) from EDX
Ni	35	29.2
Zn	15	15.4
MgO	50	34.9
O	-	20.5

EDX analysis was used to confirm the final composition of the catalyst synthesized. The elemental composition of the catalyst in weight percentages (wt%) are reported in Table S2. The EDX data of Ni-ZnO-MgO catalyst dictated that the measured Zn wt.% and the combined weight of Mg and O was aligned well with the theoretical values. However, the Ni content

measured by EDX was ~5wt.% lower than the theoretical one, which could be due to incomplete incorporation or losses of nickel during synthesis. The presence of 20.5% oxygen was consistent with the oxides.

Calculation of turnover frequency (TOF)

Turnover frequency = [Moles of CO_2 consumed/(Moles of active nickel sites × time)]

Moles of CO_2 consumed = Moles of $CO_{2,\,in}$ – Moles of $CO_{2,\,out}$

Active nickel sites = Catalyst weight (g) × Metal dispersion (%)

Moles of active nickel sites = [Active nickel metal sites (g)/Molecular weight of nickel (g/mol)]

Time = Reaction time (sec)

Table S3. **Turnover frequency (TOF) of catalysts**

Catalyst	Nickel metal dispersion (%)	Active nickel sites (g)	Moles of active nickel sites (mmol)	Turnover frequency (s^{-1})
NiO-ZnO	0.69	0.0069	0.12	0.033
NiO-MgO	1.22	0.0122	0.21	0.035
Ni-ZnO-MgO	2.54	0.0254	0.43	0.036

S.6 XPS

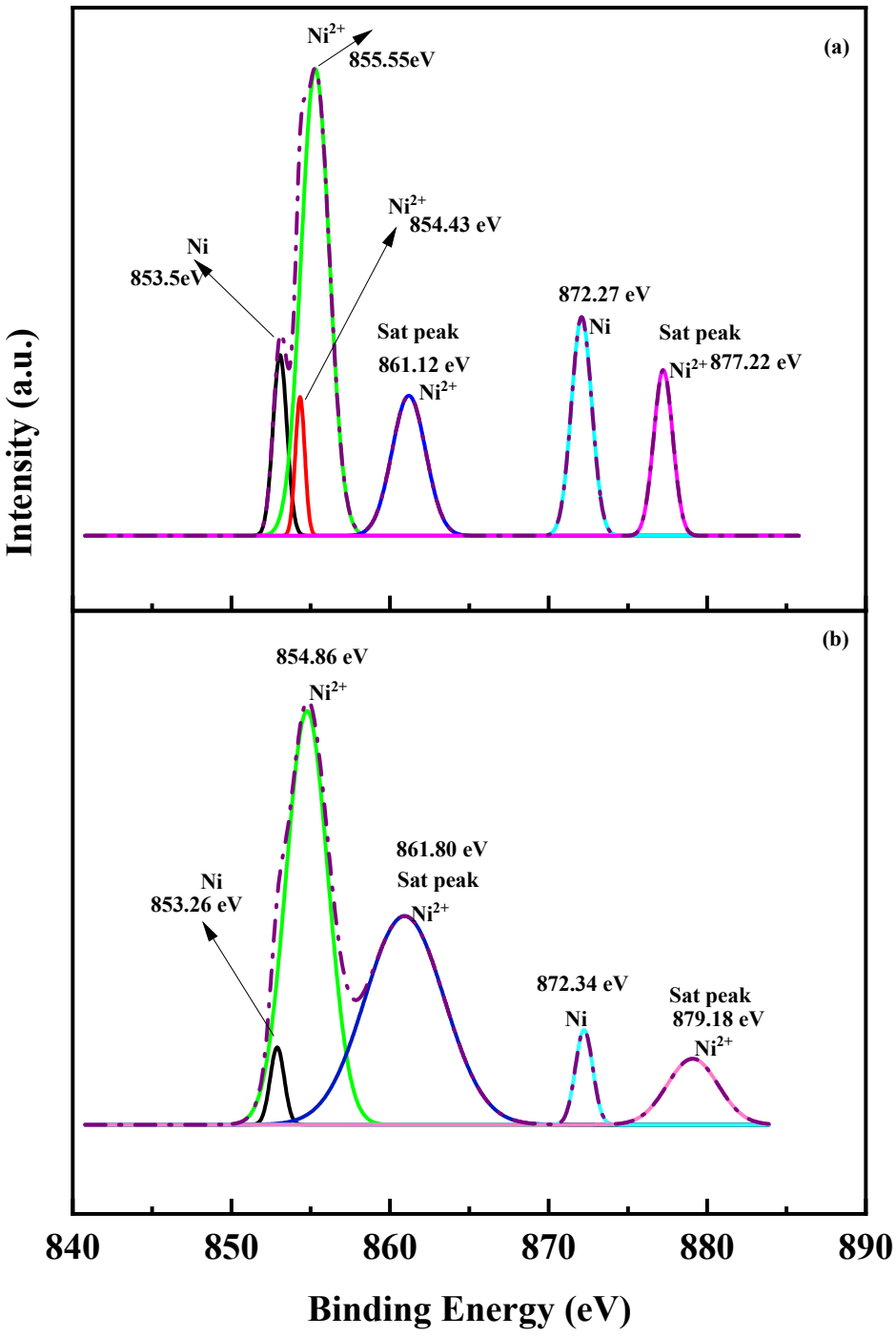

Fig. S6. 1. XPS spectra of Ni 2p (a) spent, (b) fresh reduced.

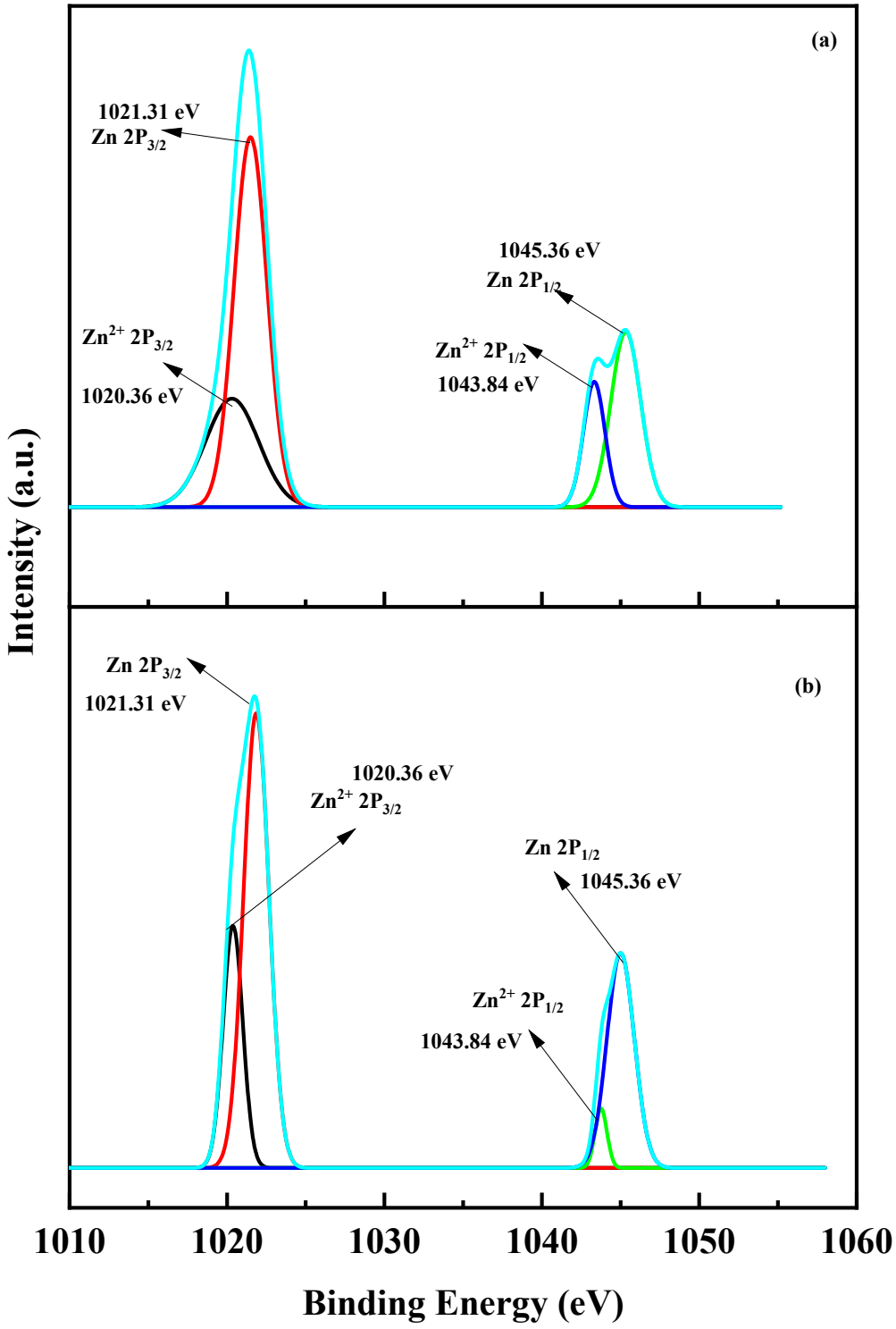

Fig. S6. 2. XPS spectra of Zn 2p (a) spent, (b) fresh reduced.

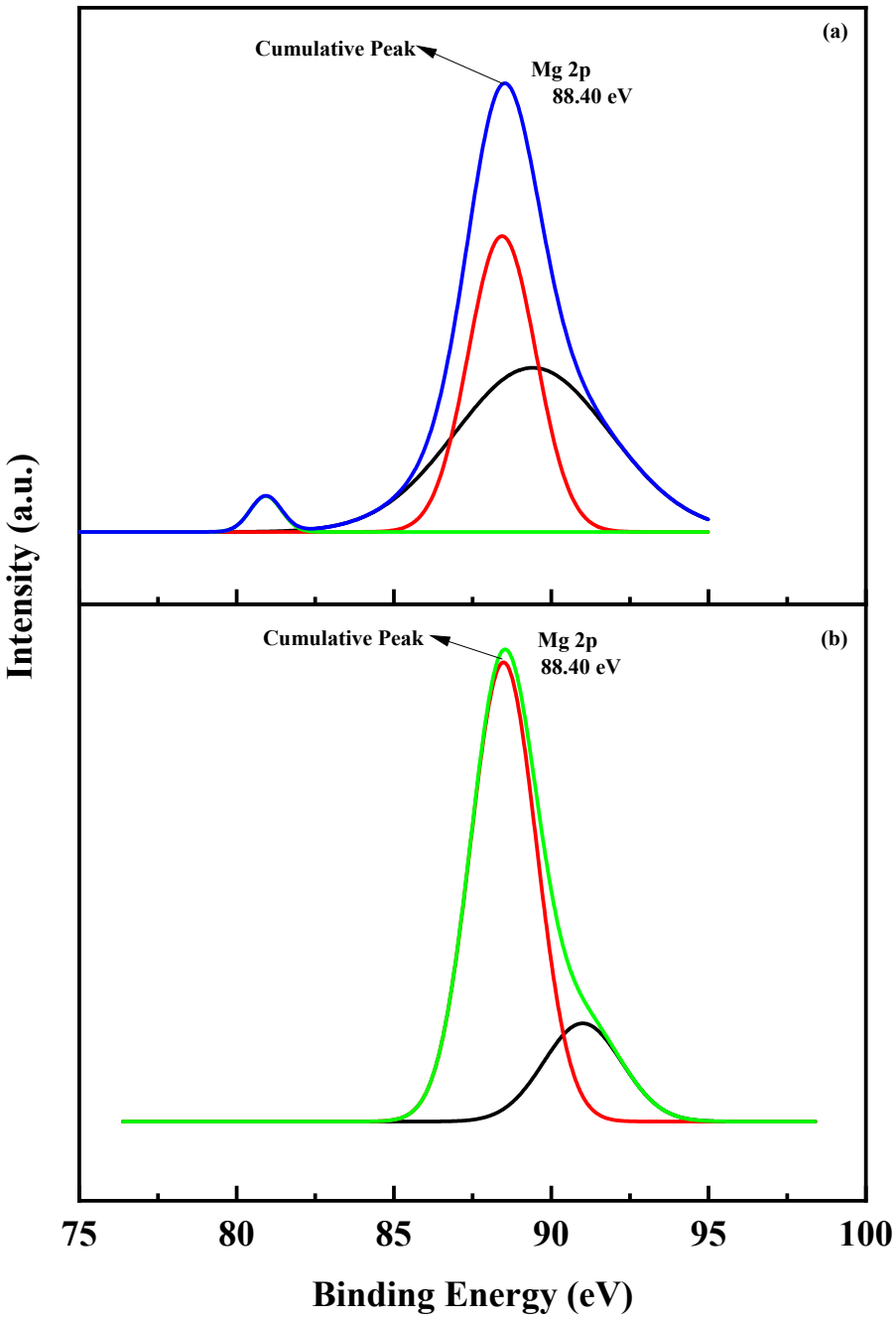

Fig. S6. 3. XPS spectra of Mg 2s (a) spent, (b) fresh reduced.

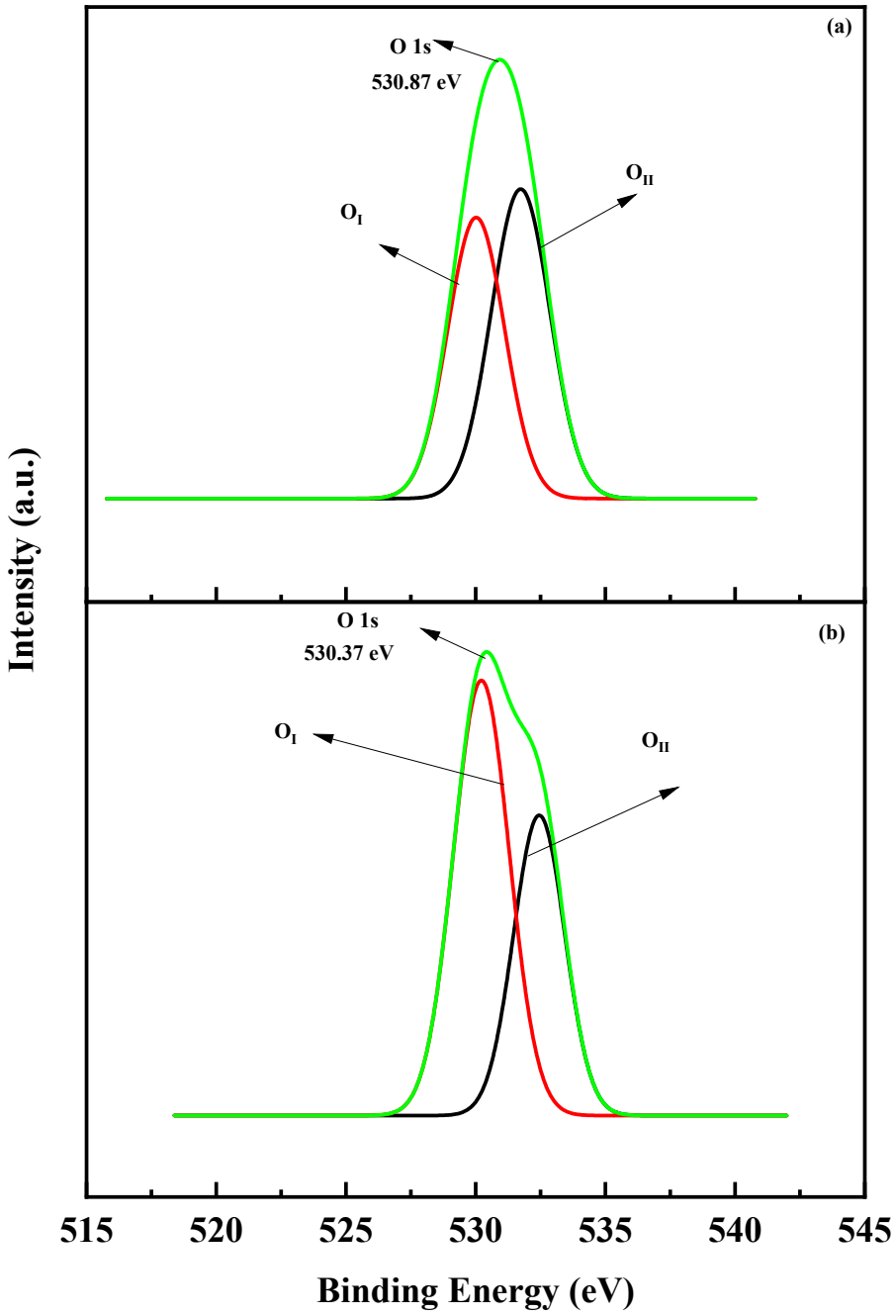

Fig. S6. 4. XPS spectra of O 1s (a) spent, (b) fresh reduced

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