

Electronic Supplementary information (ESI)

An ecofriendly route to synthesize C-Mo₂C and C/N-Mo₂C utilizing waste polyethene for efficient hydrogen evolution reaction (HER) activity and high performance supercapacitors.

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Scheme 1

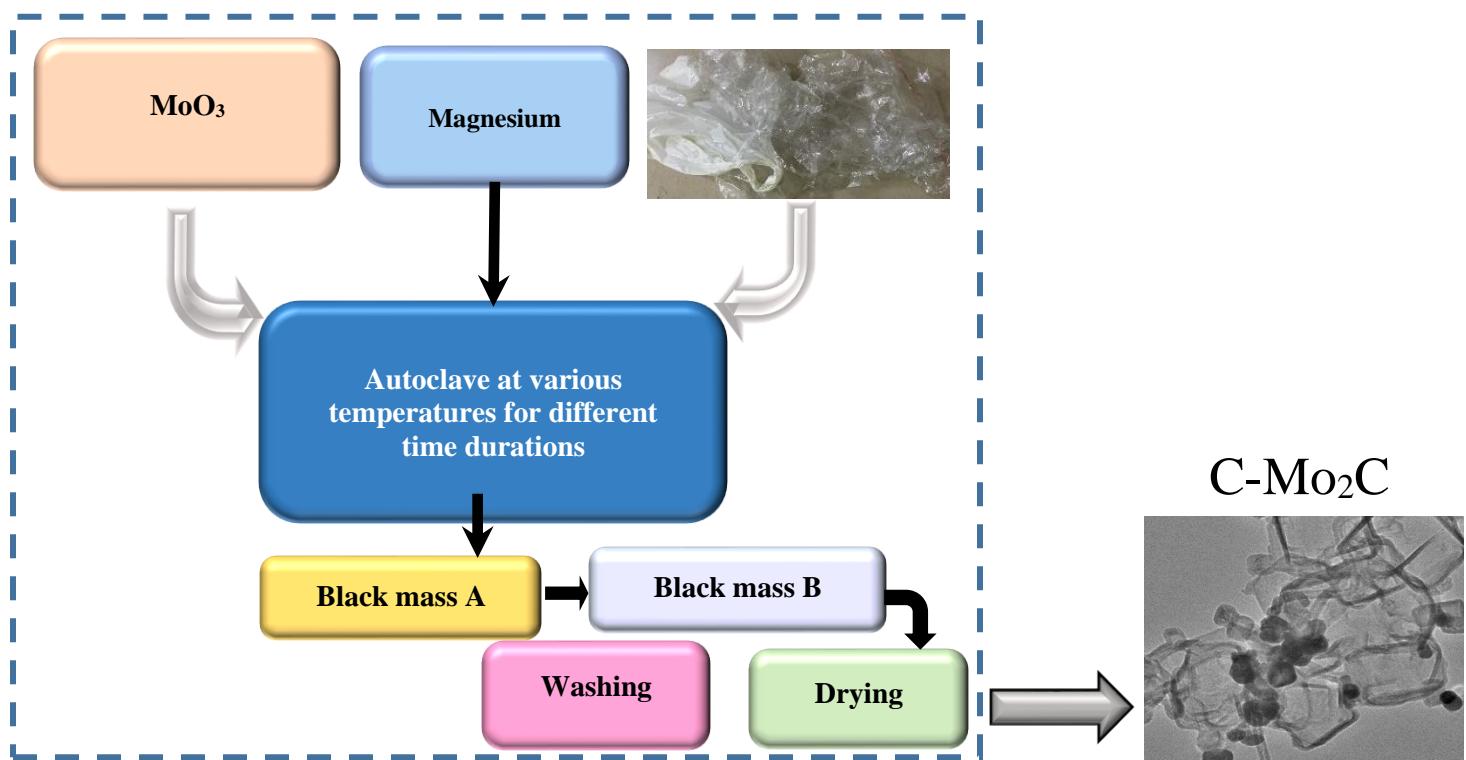


Figure S1. Experimental set for synthesis of C-Mo₂C (Scheme 1).

Scheme 2

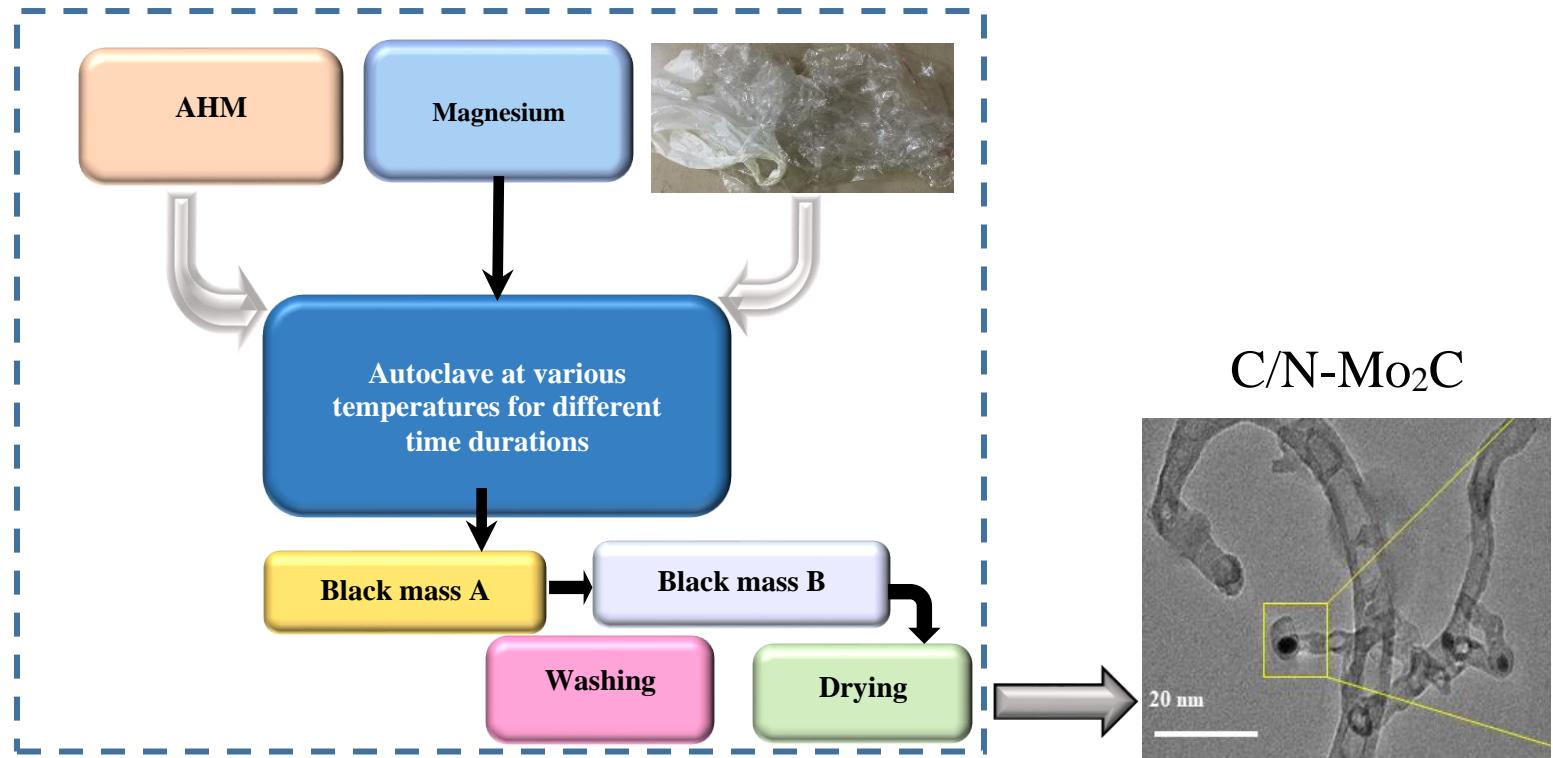


Figure S2. Experimental set for synthesis of C/N-Mo₂C (Scheme 2).

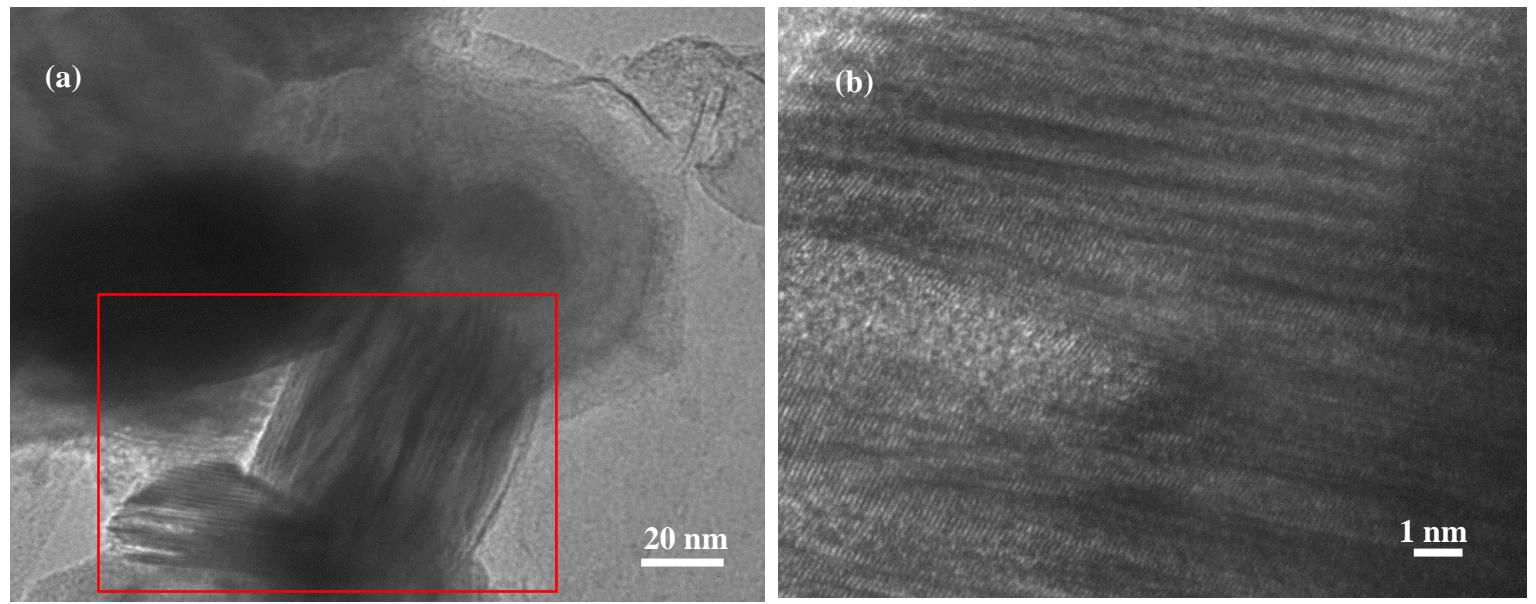


Figure S3. TEM and HRTEM micrograph of PE 600/15 showing stacking of nano structures.

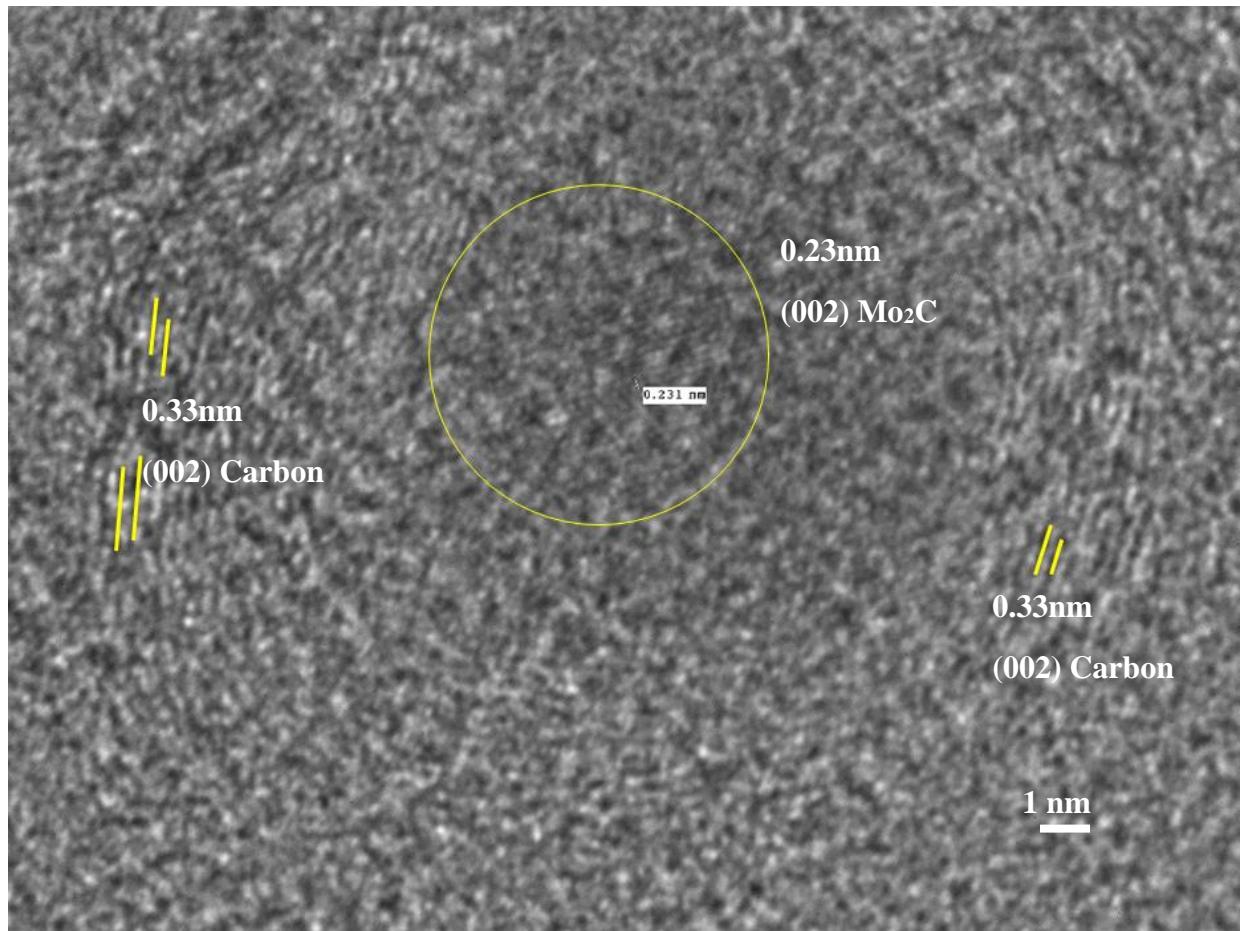


Figure S4. Magnified view of HRTEM of AMP 800/12

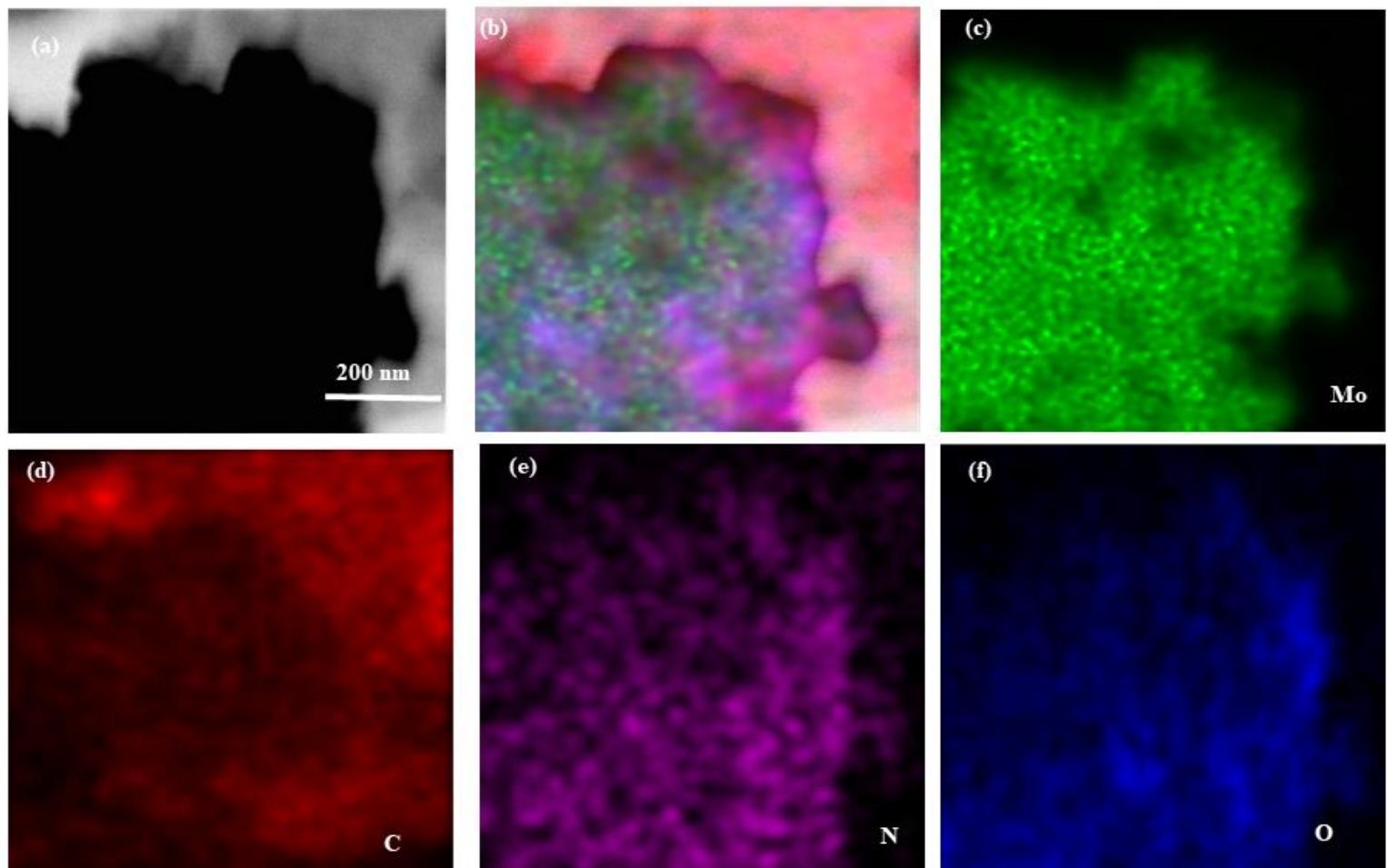


Figure S5. STEM micrograph of AMP 800/12 confirming the presence of nitrogen (N): (a) TEM micrograph, (b) survey mapping, (c) elemental molybdenum (Mo), (d) carbon (C), (e) nitrogen (N) and (f) oxygen (O).

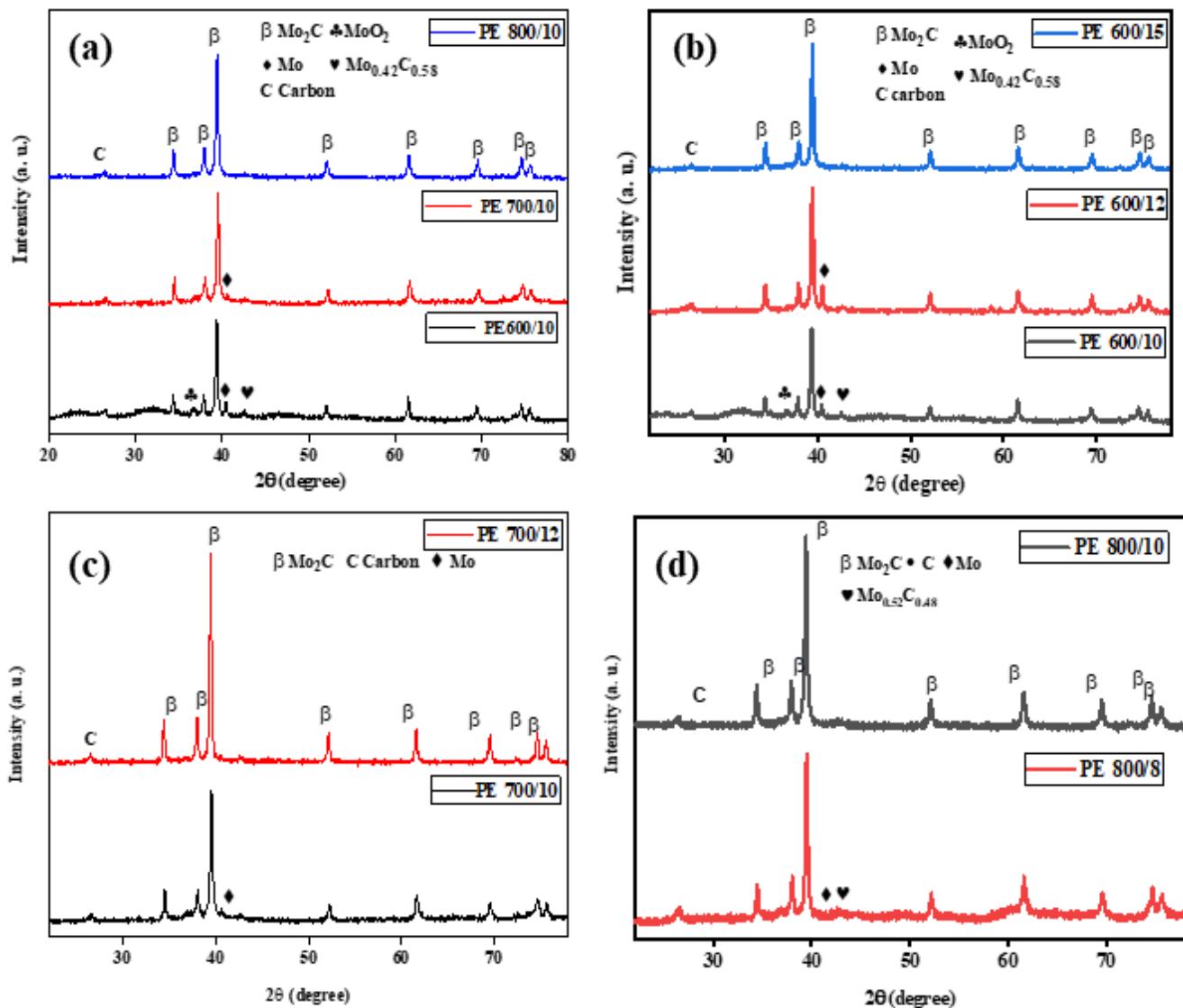


Figure S6. XRD pattern of variation of temperature and time using MoO_3 as molybdenum source (Scheme 1), (a) Variation of temperature at fixed time and variation of time at (b) 600 °C, (c) 700 °C and (d) 800 °C.

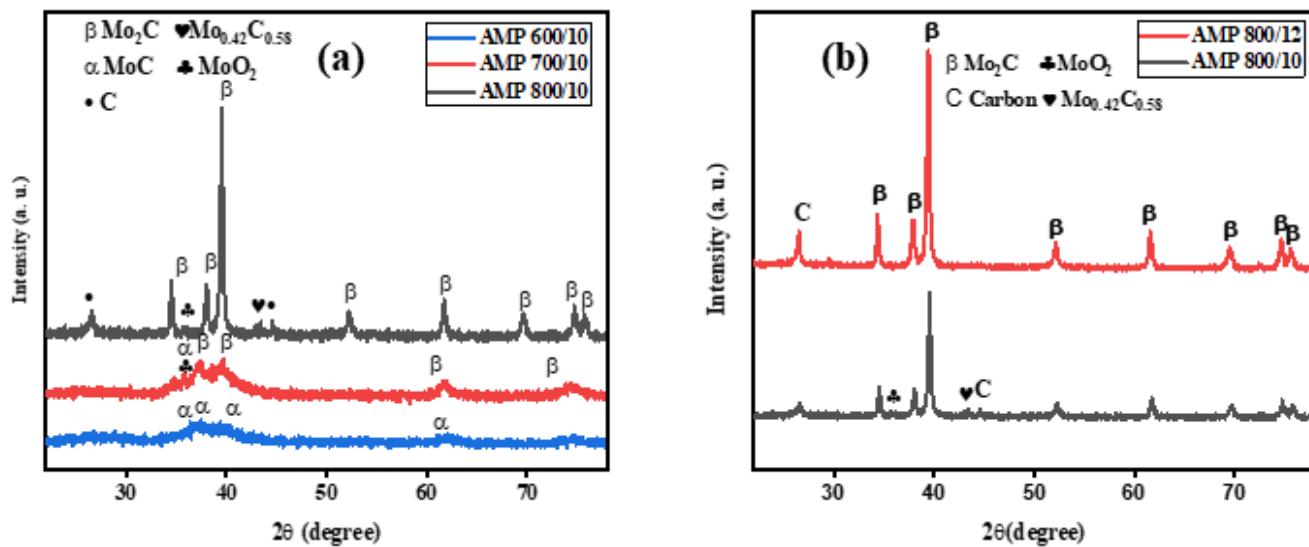


Figure S7. XRD pattern of variation of temperature and time using AHM ($(\text{NH}_4)_6\text{Mo}_7\text{O}_{24}4\text{H}_2\text{O}$) as molybdenum source (Scheme 2), (a) Variation of temperature at fixed time and (b) variation of time at 800 °C.

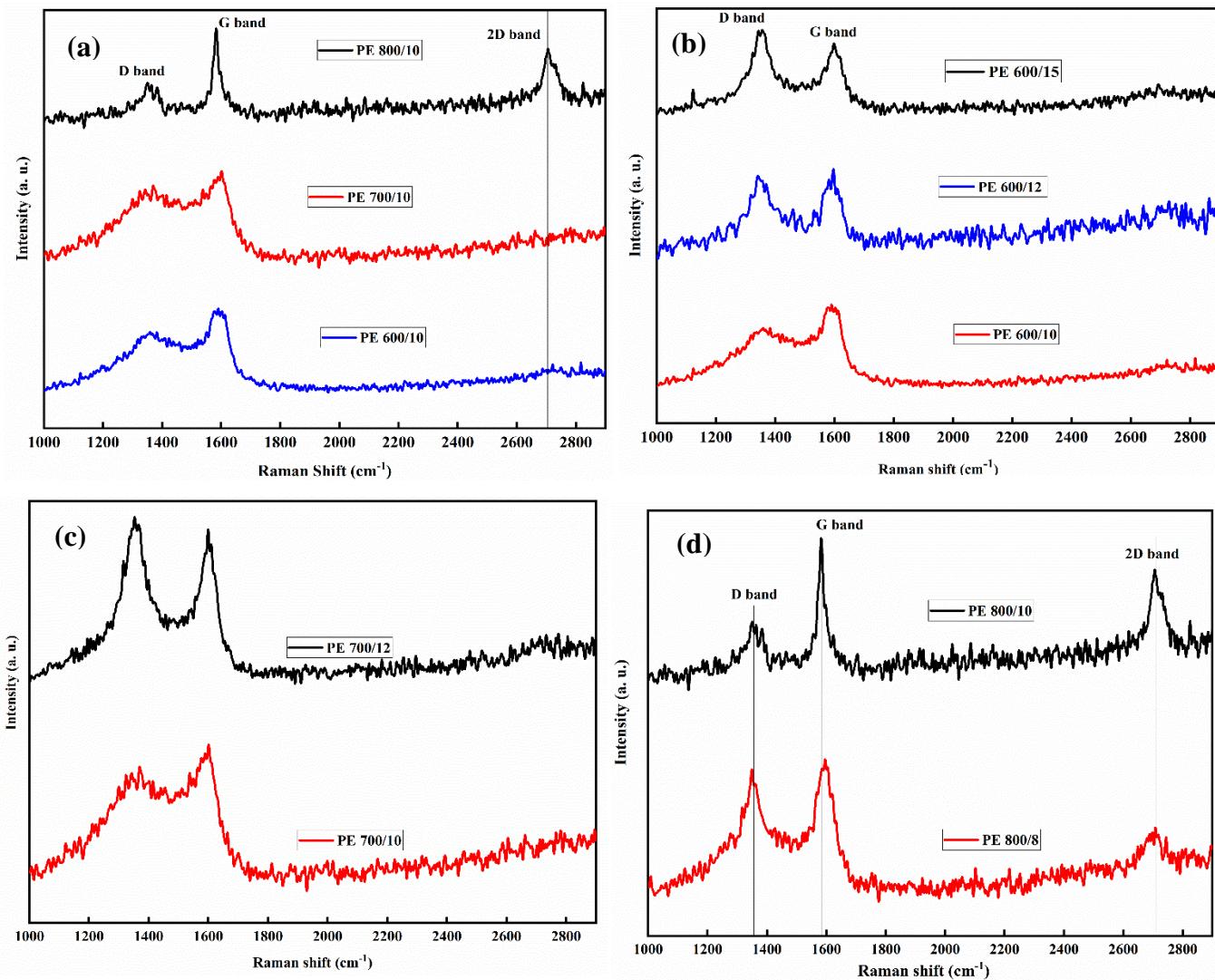


Figure S8. Raman spectroscopy results of C-Mo₂C with variation in temperature and time using MoO₃ as molybdenum source (Scheme 1), (a) Variation of temperature at fixed time and variation of time at (b) 600 °C, (c) 700 °C & (d) 800 °C.

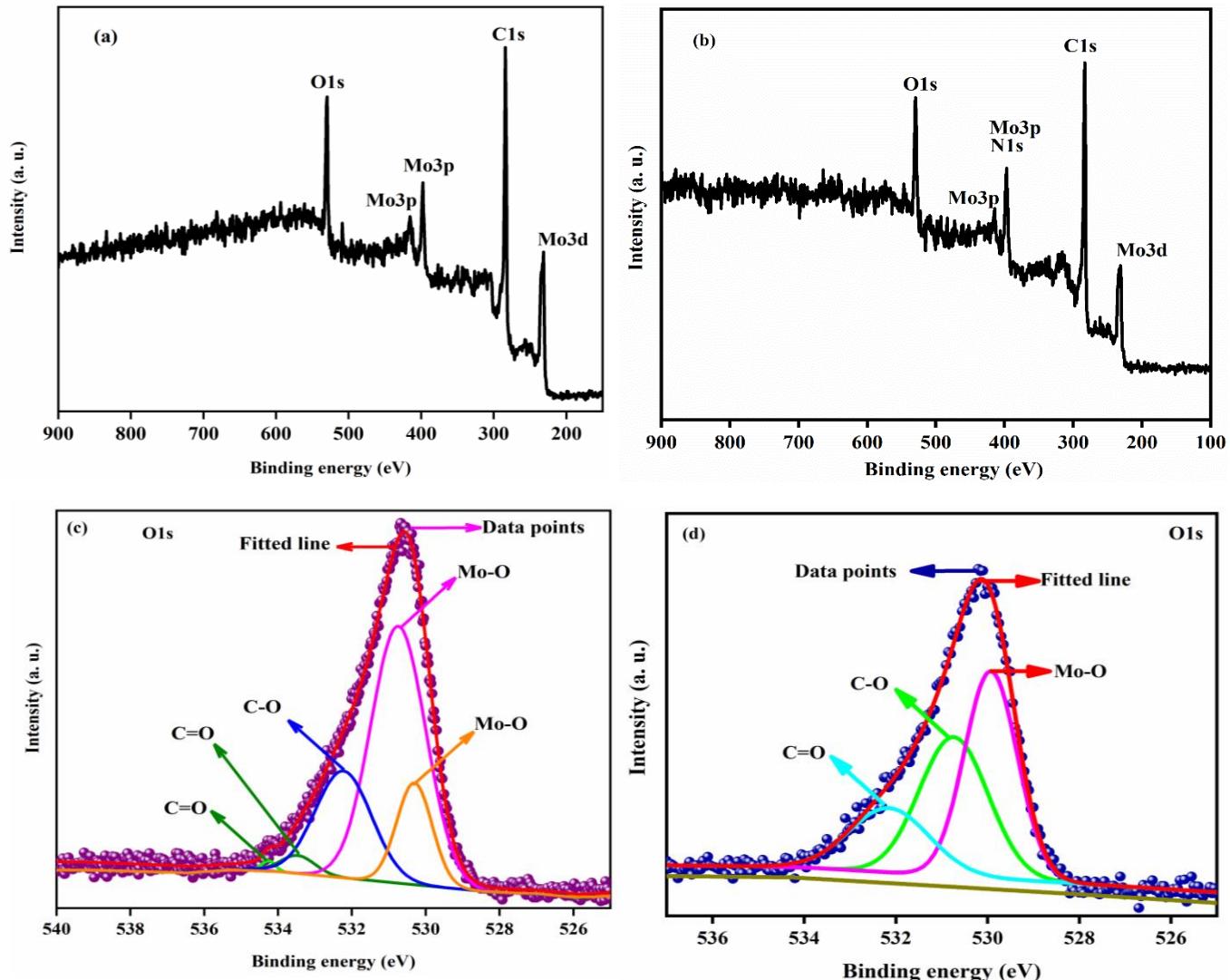


Figure S9. XPS Survey spectra of (a) PE 800/10, (b) AMP 800/12 and high resolution (HR) XPS spectra of (c) O1s (PE 800/10) and (d) O1s (AMP 800/12).

The survey spectrum of XPS represents the presence of Mo3d, C1s, Mo3p and O1s at positions (231.2 & 530.7), (284 & 283.7), (397.1 & 414.5), (529.4 & 529.5) eV for PE 800/10 and AMP 800/12, respectively. The Mo3p and N1s peak overlap at the same positions. For the nitrogen incorporated samples AMP 800/12, the N1s peak is designated at 397.6 & 414.6 eV, which can be bonding of Mo-N also at 414.6 eV.

The peak at positions (530.3 & 529.9 eV), (530.7 eV) and (532.3 and 532.2 eV) in both PE 800/10 and AMP 800/12 correspond to Mo-O and C-O, respectively. The additional peaks in PE 800/10 at 533.4 and 534.2 eV attributed to C=O, as shown in Fig. S7c.

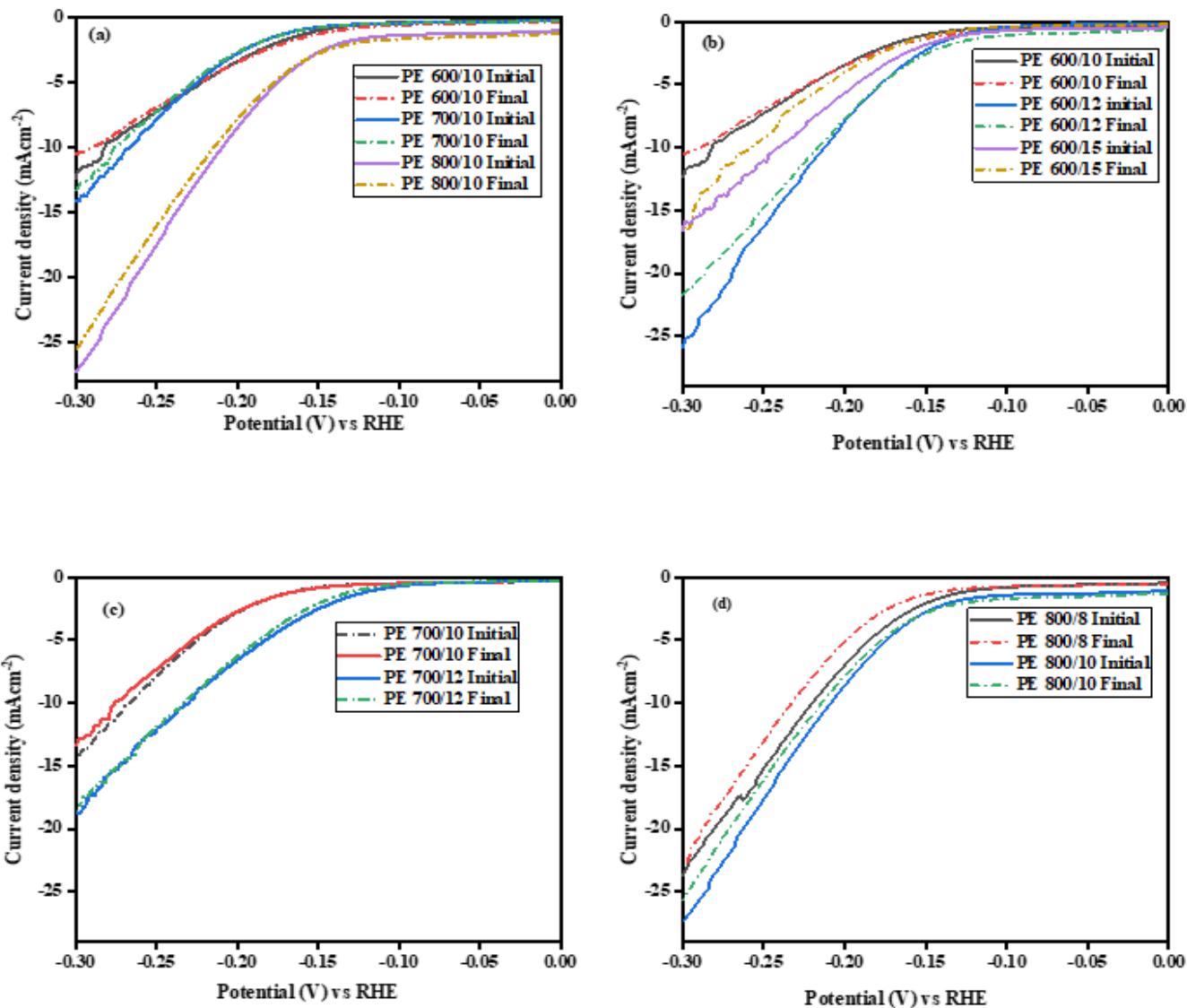


Figure S10. LSV plots of C-Mo₂C samples with respect to (a) change in temperature, and variation in reaction time at fixed temperatures at (b) 600 °C, (c) 700 °C & (d) 800 °C

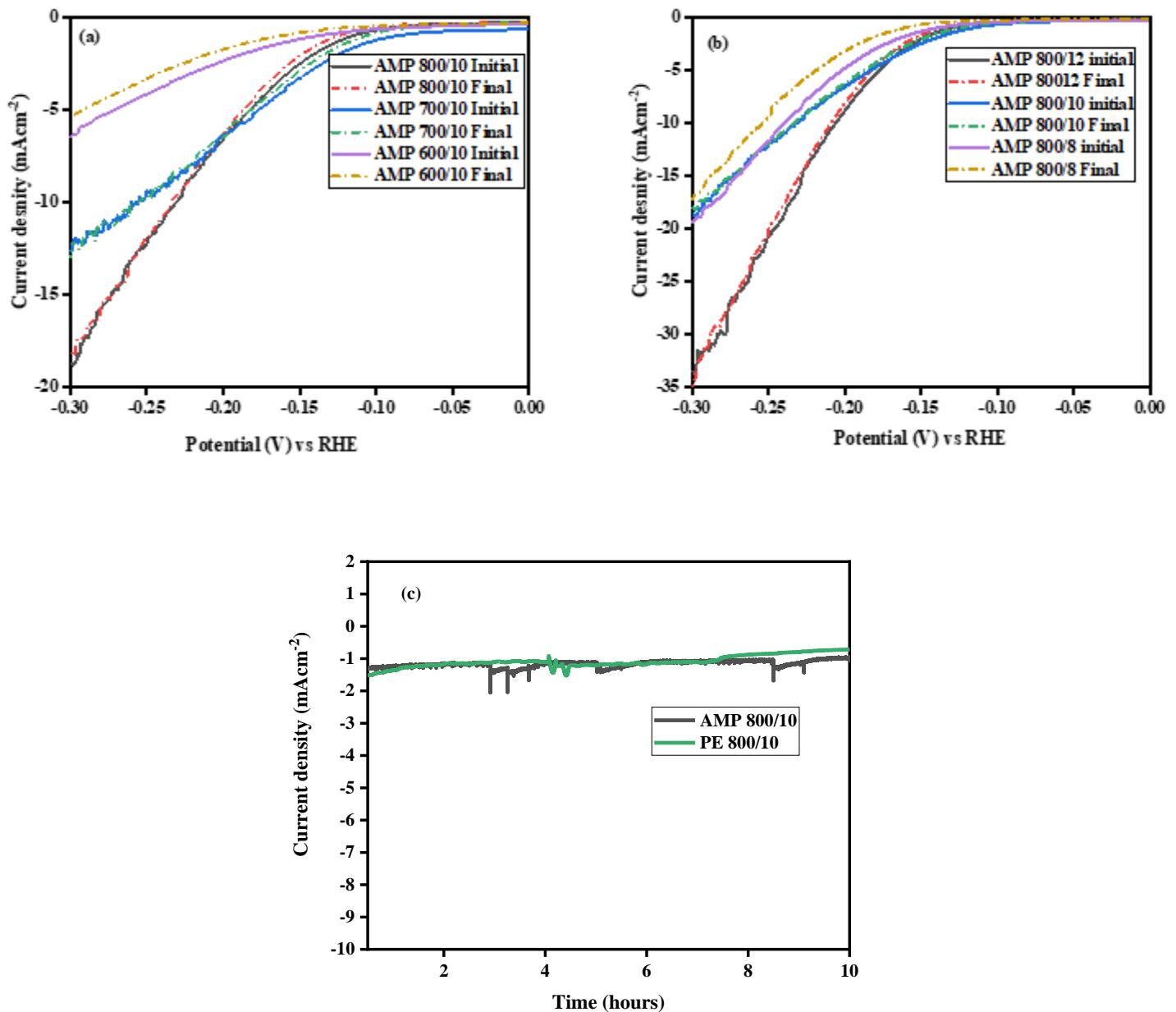


Figure S11. LSV plots of C/N-Mo₂C samples with respect to (a) change in temperature, and variation in reaction time at fixed temperatures at (b) 800 °C and (c) chronoamperometry plot of PE 800/10 and AMP 800/12.

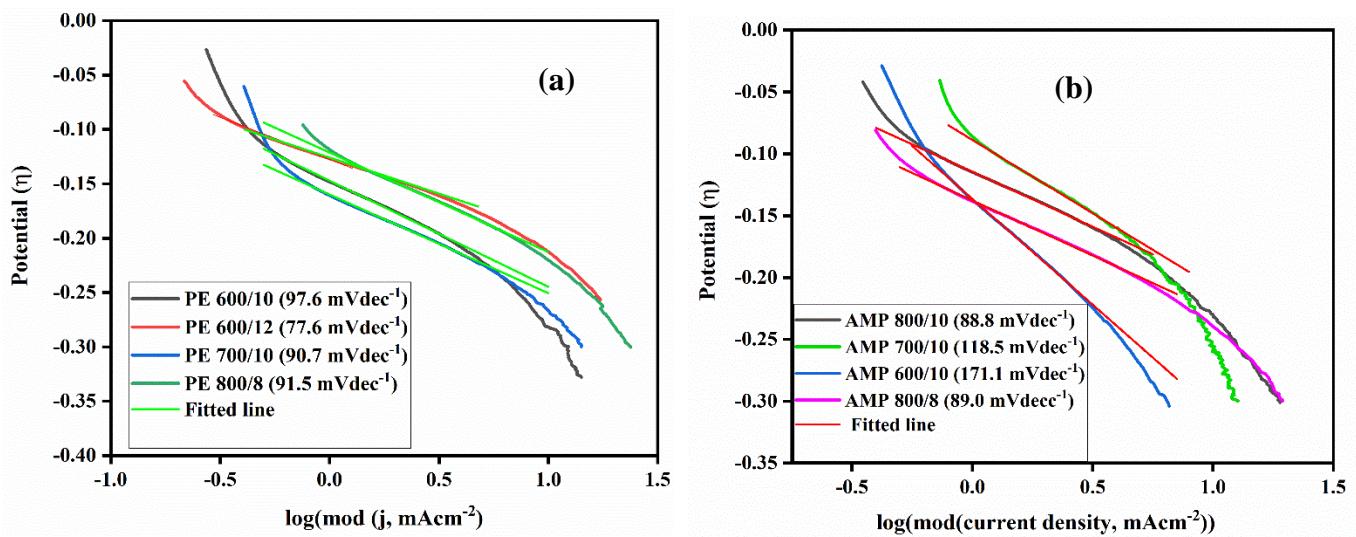


Figure S12. Tafel plots of (a) C-Mo₂C (PE 600/10, PE 600/12, PE 700/10 and PE 800/8) and (b) C/N-Mo₂C (AMP 600/10, AMP 700/10, AMP 800/10 and AMP 800/8)

Table S1. HER activity parameters, C_{dl} and SC of synthesized samples

Sample	Tafel slope (mVdec ⁻¹)	Over potential (mV) at 10 mAcm ⁻²	C_{dl} (mFcm ⁻²)	Specific capacitance (SC) Fg ⁻¹
PE 700/10	90.7	250.57	7.7	16.7
PE 600/10	97.6	244.71	13.0	28.2
PE 600/12	77.6	205.22	5.7	12.4
PE 800/8	91.5	212.67	3.5	7.6
AMP 800/10	88.8	203.3	11.7	25.4
AMP 700/10	118.5	208.2	5.2	11.3
AMP 600/10	171.1	307.46	6.3	13.6
AMP 800/8	89.0	226.67	1.9	4.1

Table S2. Comparison of HER parameters of synthesized C-Mo₂C and C/N-Mo₂C with reported results

Sample ID	Over potential (mV) at 10mAcm ⁻²	Catalyst loading (mgcm ⁻²)	Exchange Current density J ₀ (mAcm ⁻²)	Tafel Slope (mVdec ⁻¹)	Reference
PE600/15	220.5	0.461	0.054	96.0	This work
PE 700/12	206.0	0.461	0.060	91.5	
PE 800/10	197.7	0.461	0.139	71.1	
AMP 800/12	197.9	0.461	0.014	69.2	
C-Mo₂C	293	0.102	-	98	[S1]
Mo₂C/C	340			110	[27]
Mo₂C/NCNT-10	213			86	
Mo₂C/NCNT-20	200			82	
Mo₂C/NCNT-30	195			75	
Mo₂C/NCNT-40	212			81	
NCNT	497				[36]
CNT	596				
Mo₂C-nanocomposites		0.25		110-235	
Graphite				206	
P-Graphene	490			113	[56]
N-Graphene	533			116	
N,P-Graphene	422			91	
Mo₂C@NC-1	306		-	99	
Mo₂C@NC-2	240		-	83	[S2] - - - -
Mo₂C@NC-3	270		-	90	
Mo₂C@NC-4	301		-	145	
Mo₂C@NC-2-650	310		-	99	

MC-G50	283	0.33-0.357		101	[3]
MC-G100	259	0.33-0.357		93	
MC-G350	206	0.33-0.357		67	
MC-G500	216	0.33-0.357		71	
Mo₂C/CNT	251	8.2		251	[4]
Mo₂C/CNG	264	6.3		264	
Mo₂C	410		0.011	124	[S5]
Fe- Mo₂C	377		0.014	132	
Co- Mo₂C	243		0.020	89	
Ni- Mo₂C	205		0.028	81	
Cu- Mo₂C	227		0.017	84	
Ag- Mo₂C	210		0.030	83	

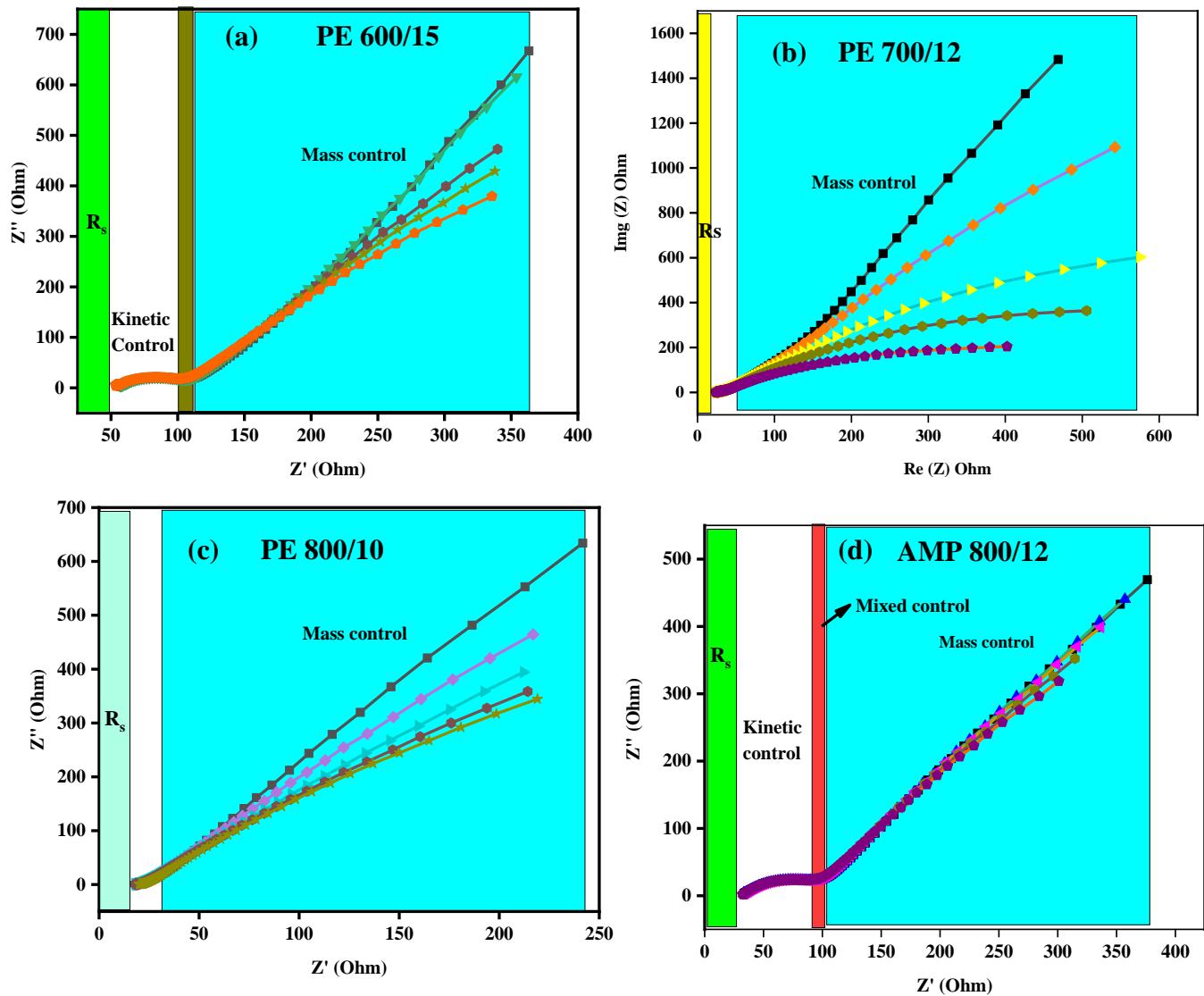


Figure S13. Nyquist plots of (a) PE 600/15, (b) PE 700/12, (c) PE 800/10 and (d) AMP 800/12

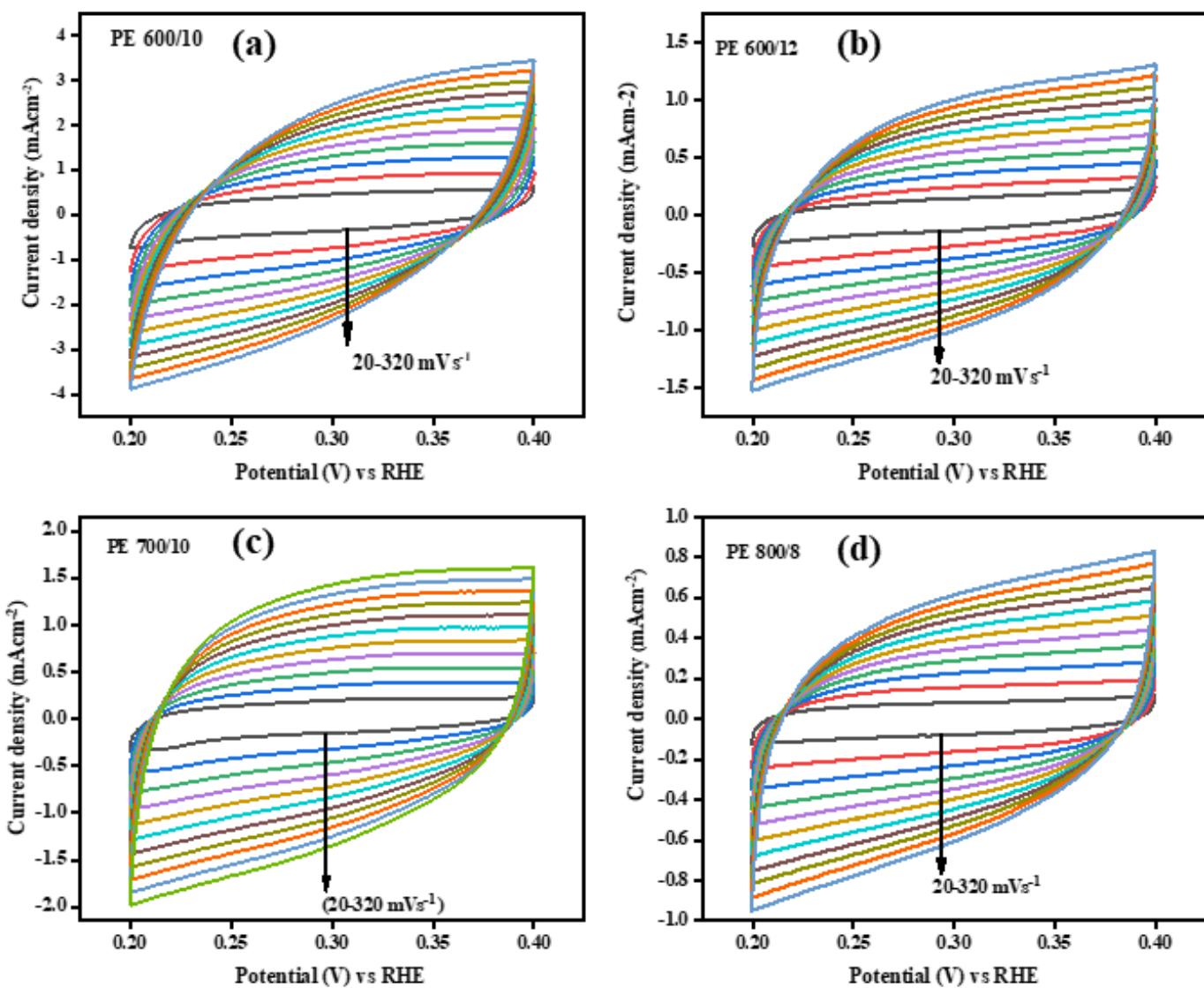


Figure S14. CV with different scan rates (a) PE 600/10, (b) PE 600/12, (c) PE 700/10 and PE 800/8

The oxide phase contained sample (PE 600/12) shows the quasi rectangular CV curve at multiple scan rates, which might correspond to some redox reaction taking place at these sites.

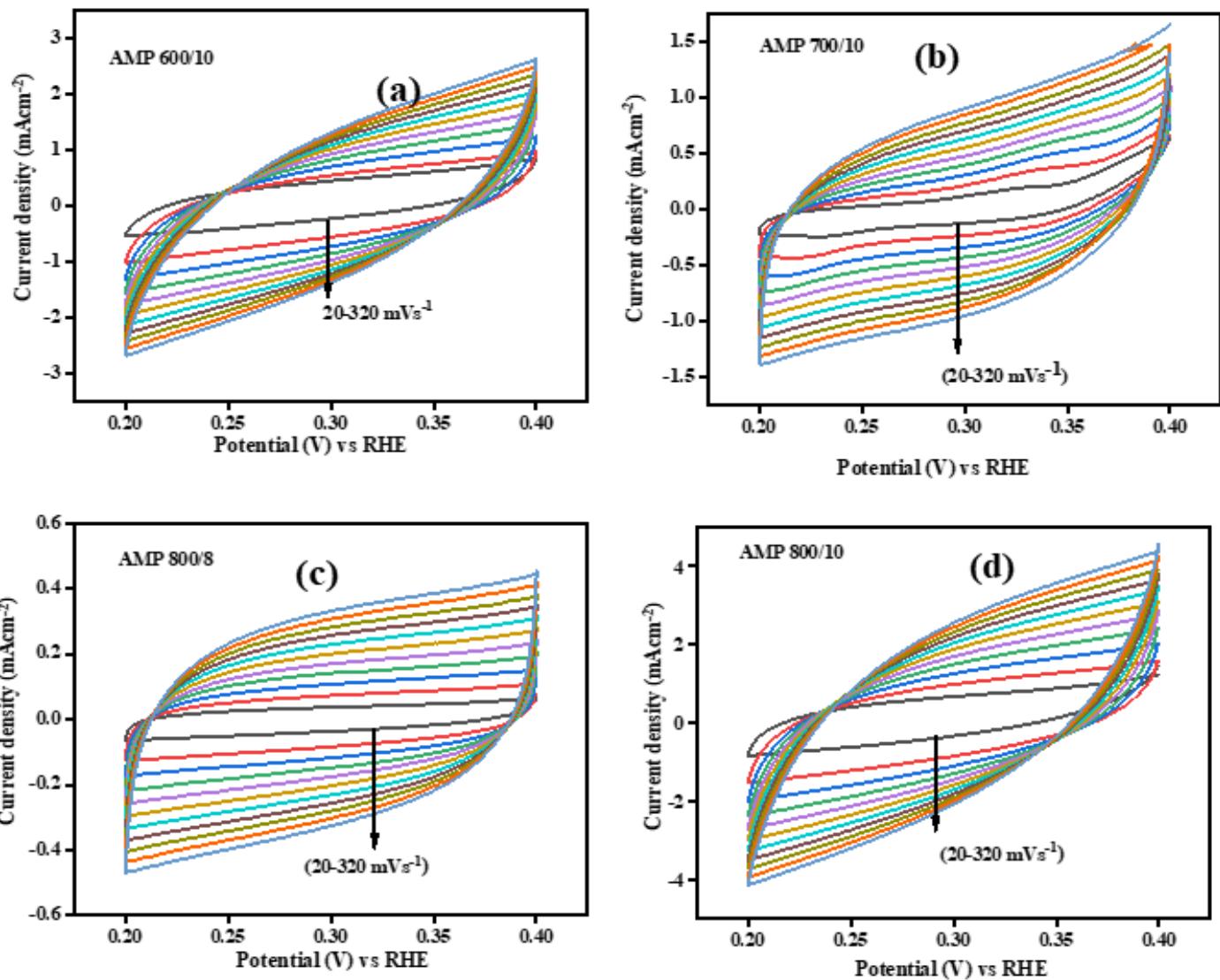


Figure S15. CV with different scan rates (a) AMP 600/10, (b) AMP 700/10, (c) AMP 800/8 and AMP 800/10

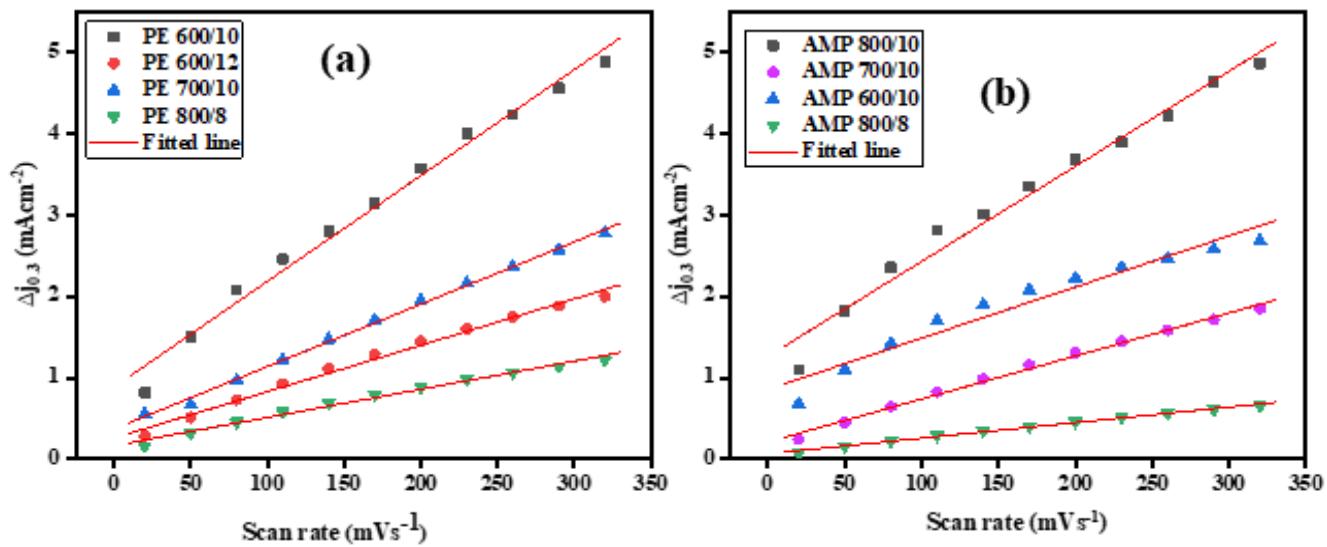


Figure S16. EDLC measurements of samples synthesized via (a) scheme 1(PE 600/10, PE 600/12, PE 700/10 and PE 800/8) and (b) scheme 2 (AMP 600/10, AMP 700/10, AMP 800/8 and AMP 800/10)

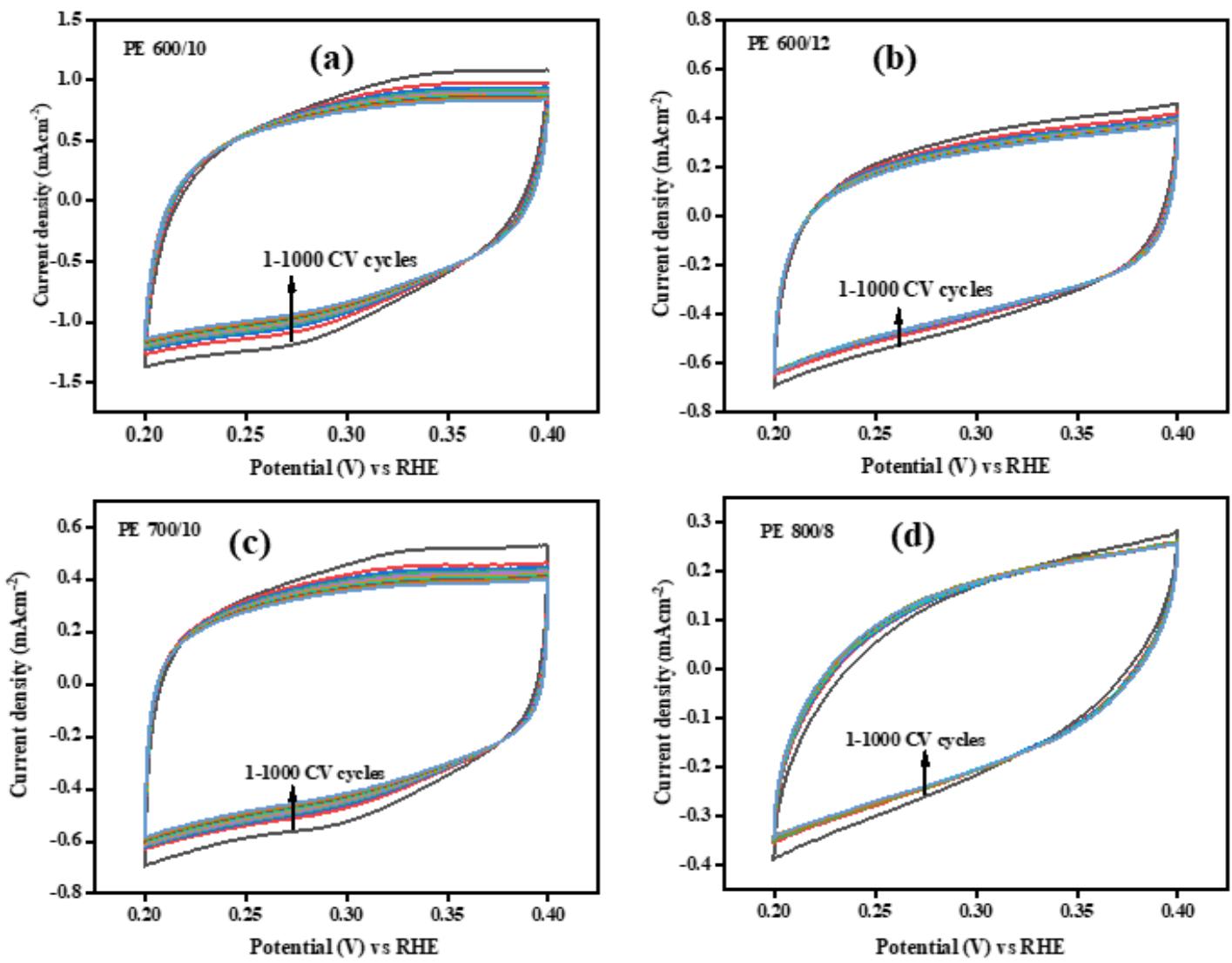


Figure S17. CV at fix scan rate for 1000 cycles (a) PE 600/10, (b) PE 600/12, (c) PE 700/10 and PE 800/8

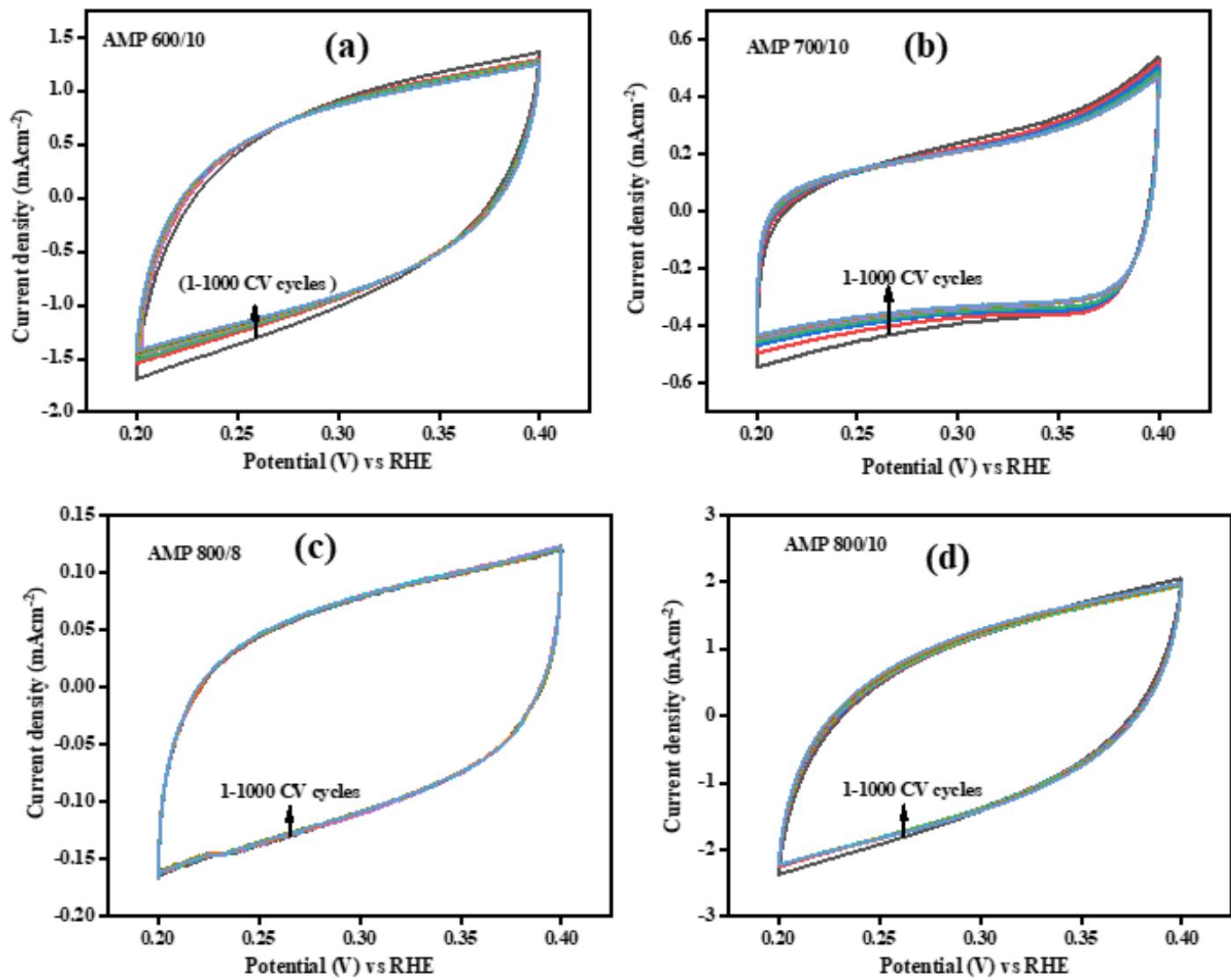


Figure S18. CV at fix scan rate for 1000 cycles (a) AMP 600/10, (b) AMP 700/10, (c) AMP 800/8 and AMP 800/10

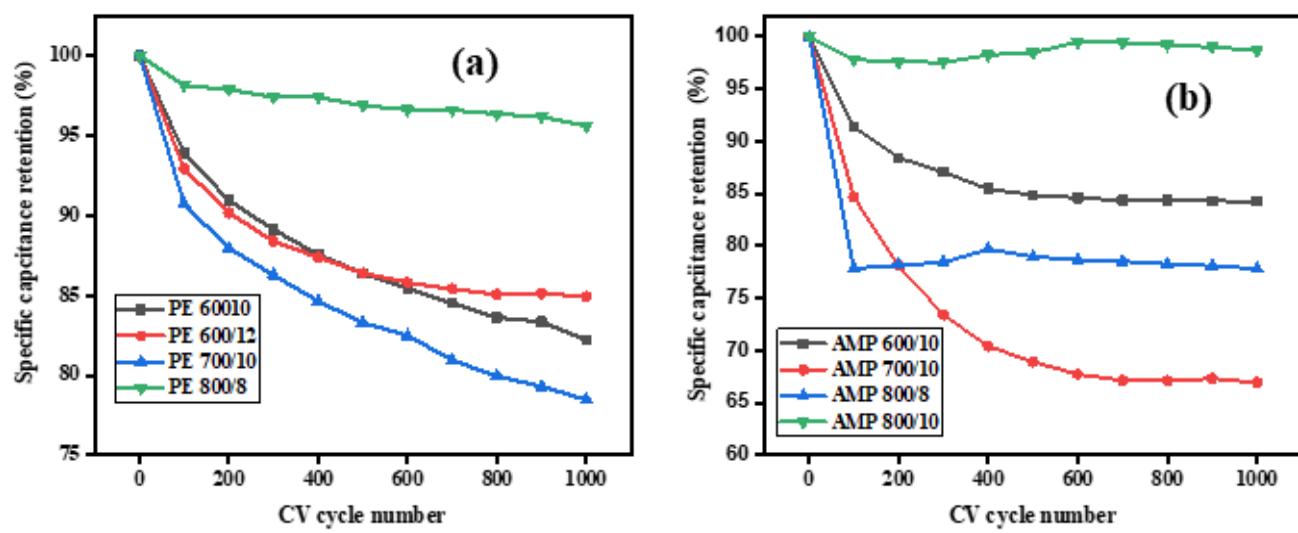


Figure S19. Specific capacitance retention (%) for samples synthesized by (a) scheme 1(PE 600/10, PE 600/12, PE 700/10 and PE 800/8) and (b) scheme 2 (AMP 600/10, AMP 700/10, AMP 800/8 and AMP 800/10)

References

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