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Sugarcane molasses as pseudocapacitive materials for supercapacitors

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Table S-1. Surface chemical composition (at.%) of the studied samples, determined by XPS1).

Sample	C	N	O	K	Ca	Na	S	Cu	Zn	Mg	Cl	Si
M-750	57.3	-	18.3	12.2	1.9	0.3	2.7	*	0.2	1.8	5.2	-
M-900	53.8	-	21.7	11.9	2.4	0.2	3.9	0.1	0.2	2.9	2.8	-
MH	83.7	0.9	13.7	-	0.4	-	0.3	-	*	1	-	-
MH-750	87.9	0.7	7.5	0.3	0.8	*	1.2	*	-	1.1	-	0.3
MH-900	85.9	0.6	7.5	0.8	1.3	*	2.2	-	*	1.5	-	-
SH	83.9	-	16.1	-	-	-	-	-	-	-	-	-
SH-900	97.7	-	2.3	-	-	-	-	-	-	-	-	-

1)A high K amount (~ 12 at.%) was found in M-750 and M-900, and Na was also found but at a minor concentration (~ 0.2 at.%). A small amount of Si was detected for MH-750 and > 1 at.% Mg was measured in all the molasses-derived carbons. Analysis of the Mg2p peak (Mg1s peak was not analysed because it overlapped with Auger peak of chlorine) indicated that Mg was not in the form of sulphates.

*Concentration < 0.1 at.%; (-) Non detected element.

Table S-2. Binding energy (BE) and relative area contributions to the S2p peak.

Sample	BE (eV)				A (%)	
	Oxidised		Sulphided		Oxidised	Sulphided
	$S2p_{1/2}$	$S2p_{3/2}$	$S2p_{1/2}$	$S2p_{3/2}$		
M-750	170.0	168.9	164.6	163.5	87.8	12.2
M-900	170.4	169.3	164.4	163.4	97.7	2.3
MH-750	170.2	169.0	167.9	163.8	60.1	39.9
MH-900	170.5	169.3	165.1	163.9	75.3	24.7

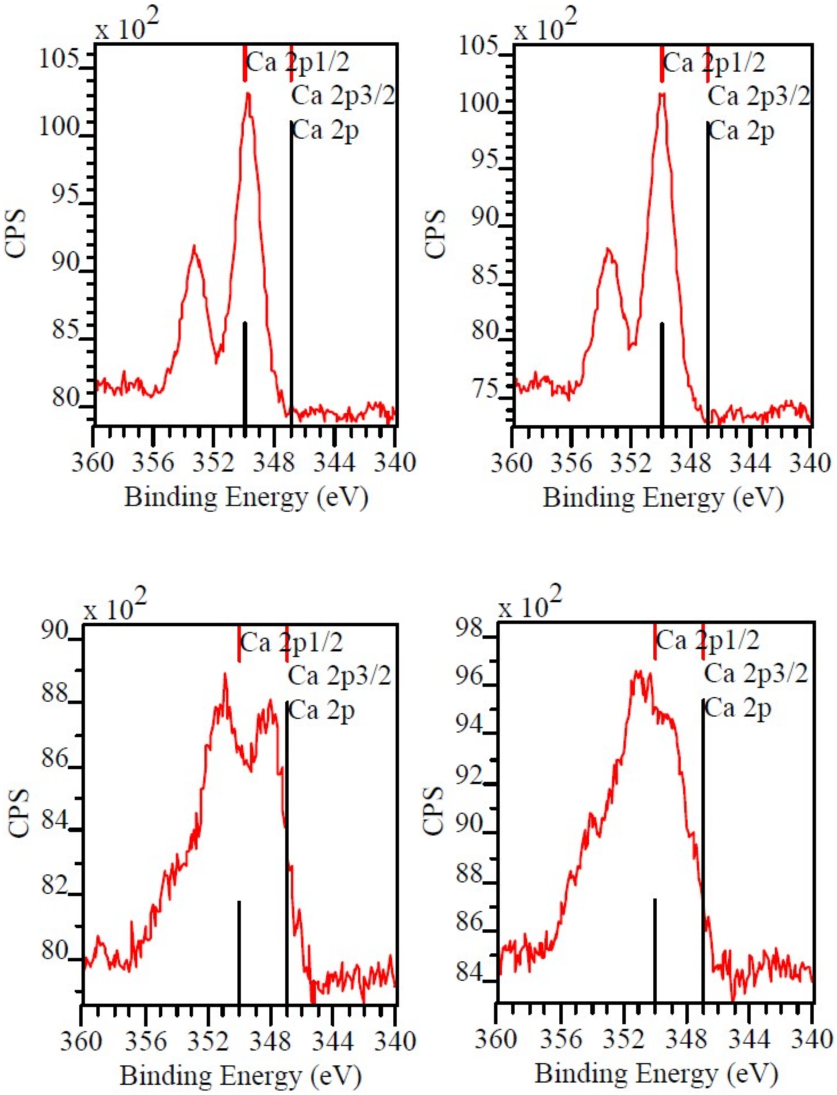


Figure S-1. XPS profiles in the Ca 2p region of the carbon materials derived from molasses. The Ca2p peak clearly exhibited spaced spin-orbit components, the spacing value between the 1/2 and 3/2 orbitals being ~ 3.5eV. This peak was centred at 347.3 and 350.9 eV, indicating that Ca was in the form of CaO and $CaSO_4$. CaO may originate from $CaCO_3$ by: i) thermal decomposition at temperatures above ~ 750°C,[28] and ii) degradation under prolonged X-ray exposure used in XPS analysis.[29] In both cases, CO_2 was produced and might be involved in the porosity development of the carbons.

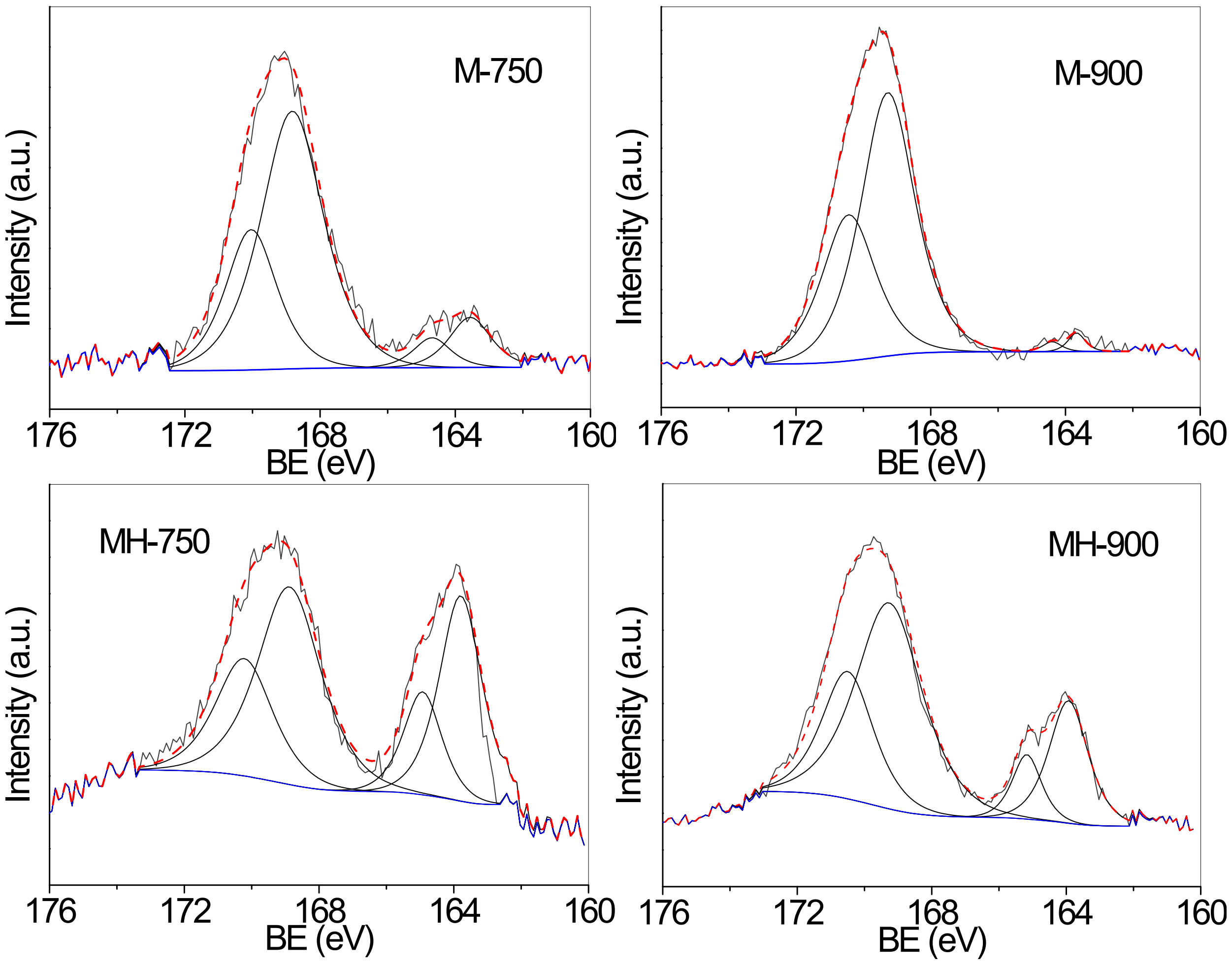
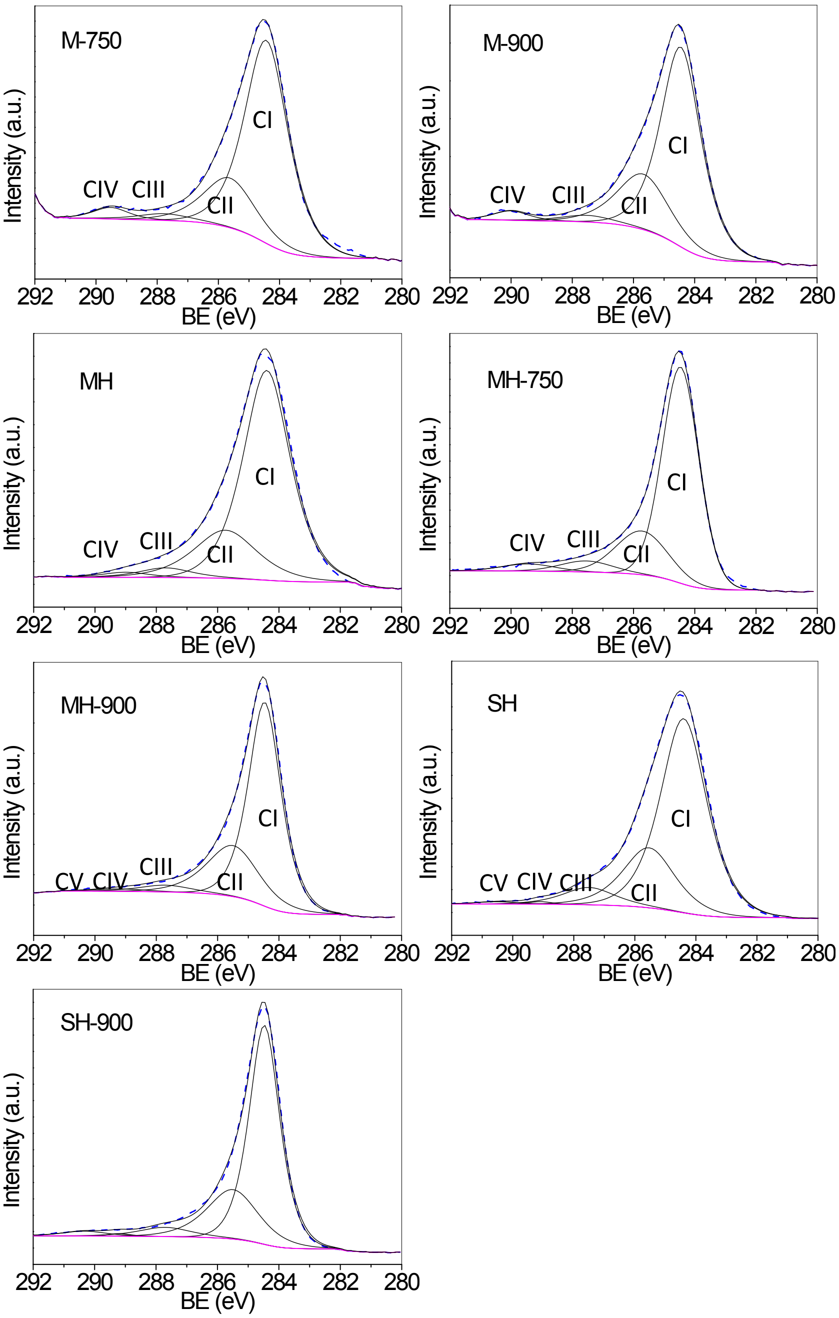


Figure S-2. S2p high-resolution spectra of the carbons materials derived from molasses. The S2p peak presented closely spaced spin-orbit components, 1.16 eV apart. No splitting between components was observed and an asymmetric peak appeared due to an unresolved doublet. The 2p orbital intensity ratio had a value of 0.51, which can be considered as appropriate because within the interval 0.48 - 0.51.



CI

CIV CIII CII

Figure S-3. C1s high-resolution spectra of the carbons materials derived from molasses. The peaks are assigned to: CI (hydrocarbons, aromatics, aliphatics), CII (single bond C-O associated to ethers, phenols and anhydrides, Csp^3, C≡N groups and C-N bonds in aromatic rings), CIII (double bond C=O in carbonyls and quinones and C=N groups), CIV (C-O bonds in carboxyls and CO-N-CO – like groups) and CV (plasmon loss or shake-up satellite π–π^*).[35]

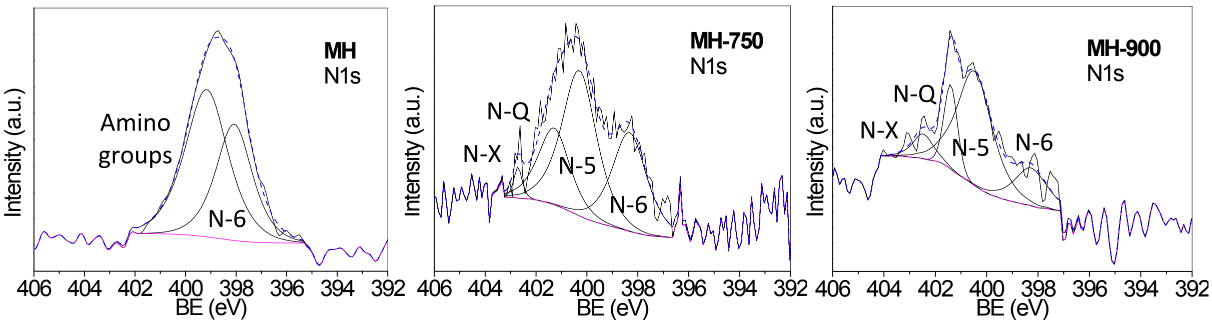


Figure S-4. N1s high-resolution spectra of the samples derived from molasses by HTC. Peak fitting displayed the presence of two nitrogen contributions for MH (N-6 and amino groups) and four contributions for MH-750 and MH-900 (N-6, N-5, N-Q and N-X). The peaks are assigned to: N-6 (pyridinic nitrogen), amino groups, N-5 (pyrrolic nitrogen), N-Q (quaternary nitrogen) and N-X (oxidised N).[35,36]

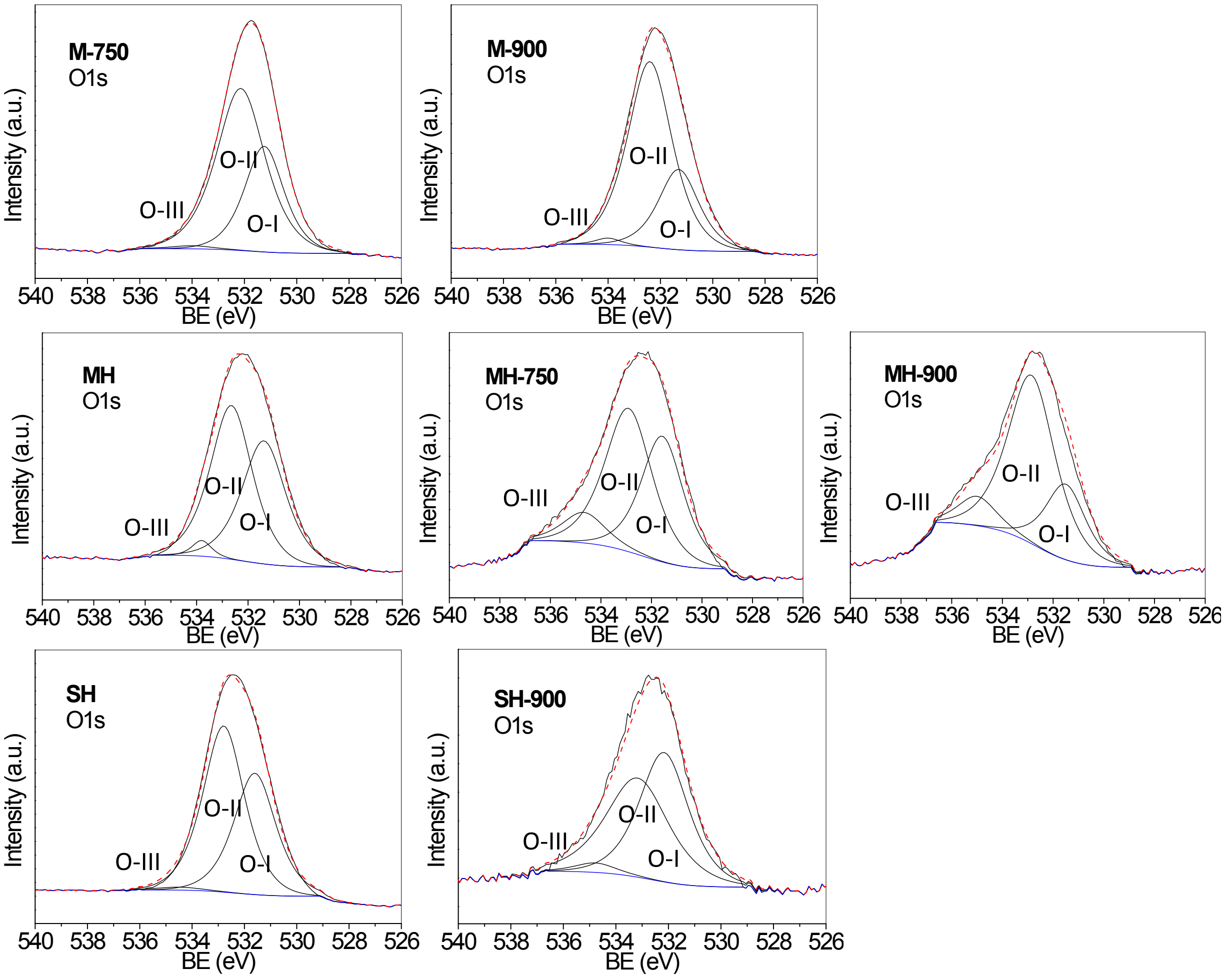


Figure S-5. O1s high-resolution spectra of the studied samples. Three contributions were obtained from the fitting of each peak: OI (C=O linkages in quinone-type groups and carbonyls), OII (–OH bonds in phenols, C–O–C ether groups and C=O bonds in ester and anhydride groups) and OIII (chemisorbed oxygen, non-carbonylic C-O bonds in esters and anhydrides, carboxylic groups and/or water).[35-37]

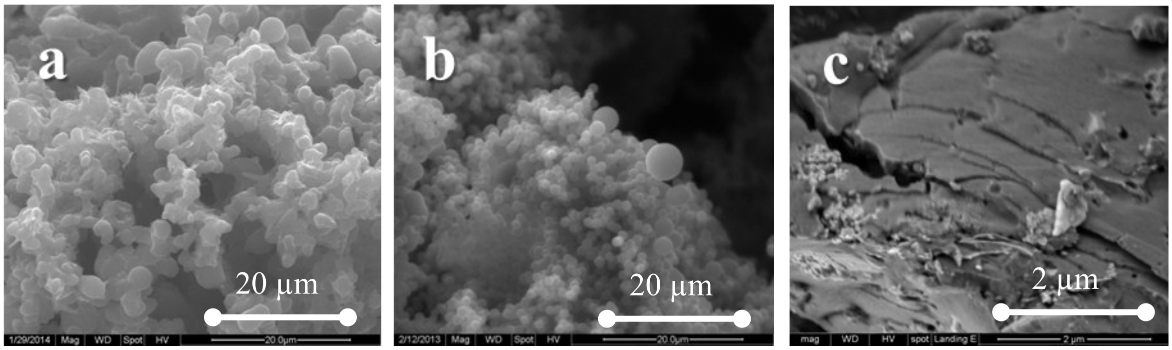


Figure S-6. SEM images of molasses- and sucrose-based carbons: (a) MH-900, (b) SH-900 and (c) M-900.

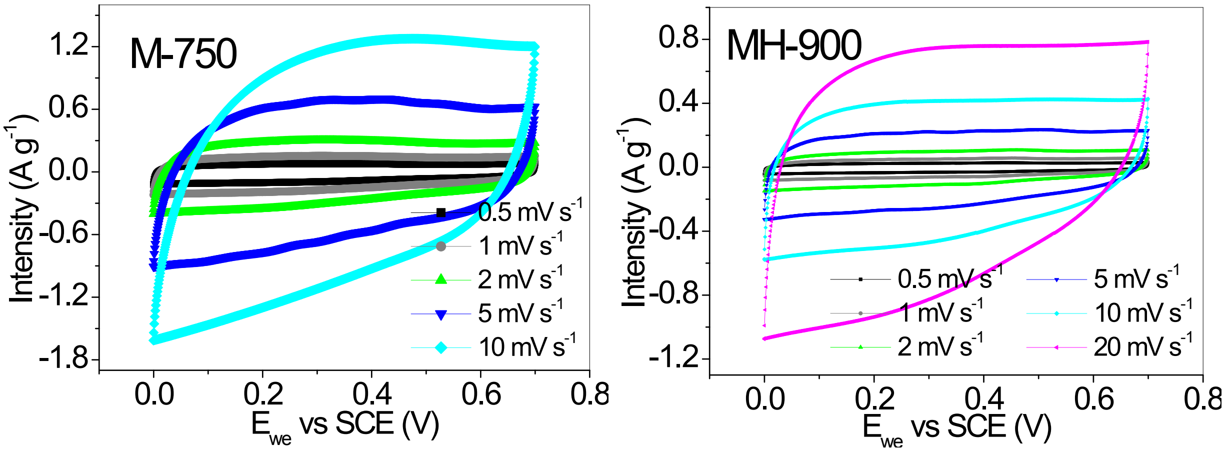


Figure S-7. CV curves of M-750 (left) and MH-900 (right) at different scan rates within the potential window 0 – 0.7 V.

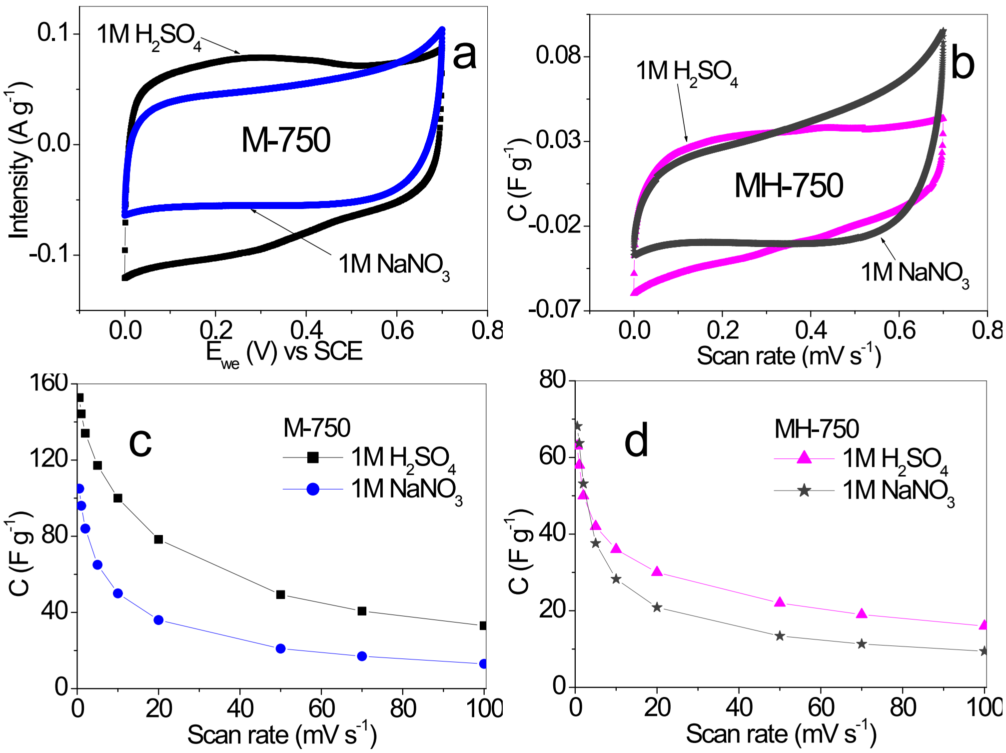


Figure S-8. CV curves obtained for M-750 (a) and MH-750 (b) in 1M H_2SO_4 or 1M $NaNO_3$ electrolytes at 0.5 mV s^{-1} scan rate. Specific capacitance results obtained in both electrolytes at different scan rates (c and d). Potential window= 0 – 0.7 V.