The impact of templating and macropores in hard carbons on their properties as negative electrode materials in sodium-ion batteries

Supporting Information

Sofiia Prykhodska[a], Konstantin Schutjajew[a], Erik Troschke[a], Leonid Kaberov[b,c], Jonas Eichhorn[b,c], Felix H. Schacher[b,c,d], Francesco Walenszus[e], Daniel Werner[f], Martin Oschatz[a,d,]*

a. Friedrich-Schiller-University Jena, Institute for Technical Chemistry and Environmental Chemistry, Philosophenweg 7a, 07743 Jena, Germany.

b. Institute of Organic Chemistry and Macromolecular Chemistry (IOMC), Friedrich Schiller-University Jena, Humboldtstraße 10, D-07743 Jena, Germany.

c. Jena Center for Soft Matter (JCSM), Friedrich Schiller University Jena, Philosophenweg 7, 07743 Jena, Germany.

d. Center for Energy and Environmental Chemistry Jena (CEEC Jena), Philosophenweg 7a, 07743 Jena, Germany.

e. 3P INSTRUMENTS GmbH & Co. KG, Bitterfelder Str. 1-5, 04129 Leipzig, Germany.

f. Max Planck Institute of Colloids and Interfaces, Department of Colloid Chemistry, Am Mühlenberg 1, 14476 Potsdam, Germany.

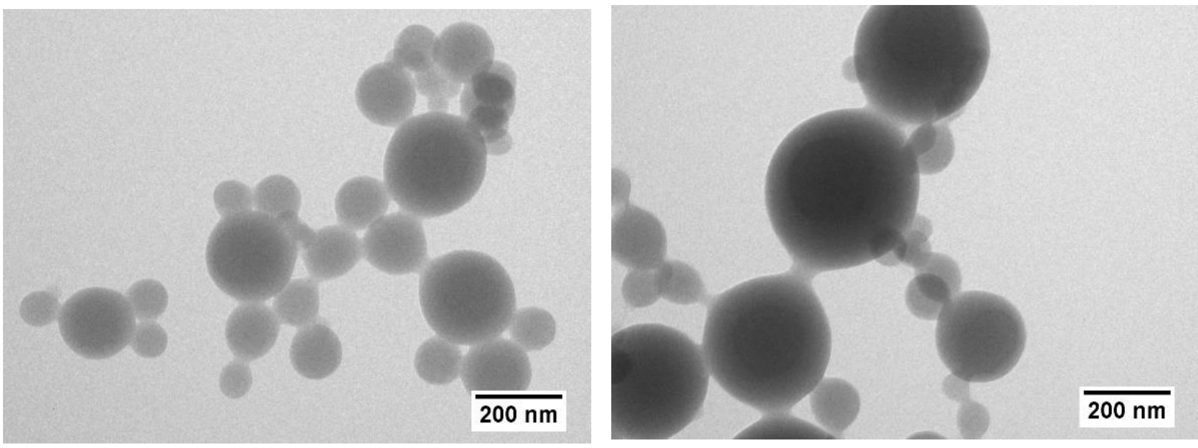

Figure S1. Transmission electron microscopy (TEM) images of polystyrene spheres.

Table S1. 2*θ* position of (002) and (100) reflections as well as full width at half maximum (FWHM) from PXRD of hard carbon materials.

	2*θ* (002), °	**2*θ* (100), °**	**FWHM (002)**	**FWHM (100)**
PS-HC-2	23.55	43.90	5.69	3.81
PS-HC-20	23.92	44.04	5.59	4.19
HC	23.90	44.04	5.99	4.11

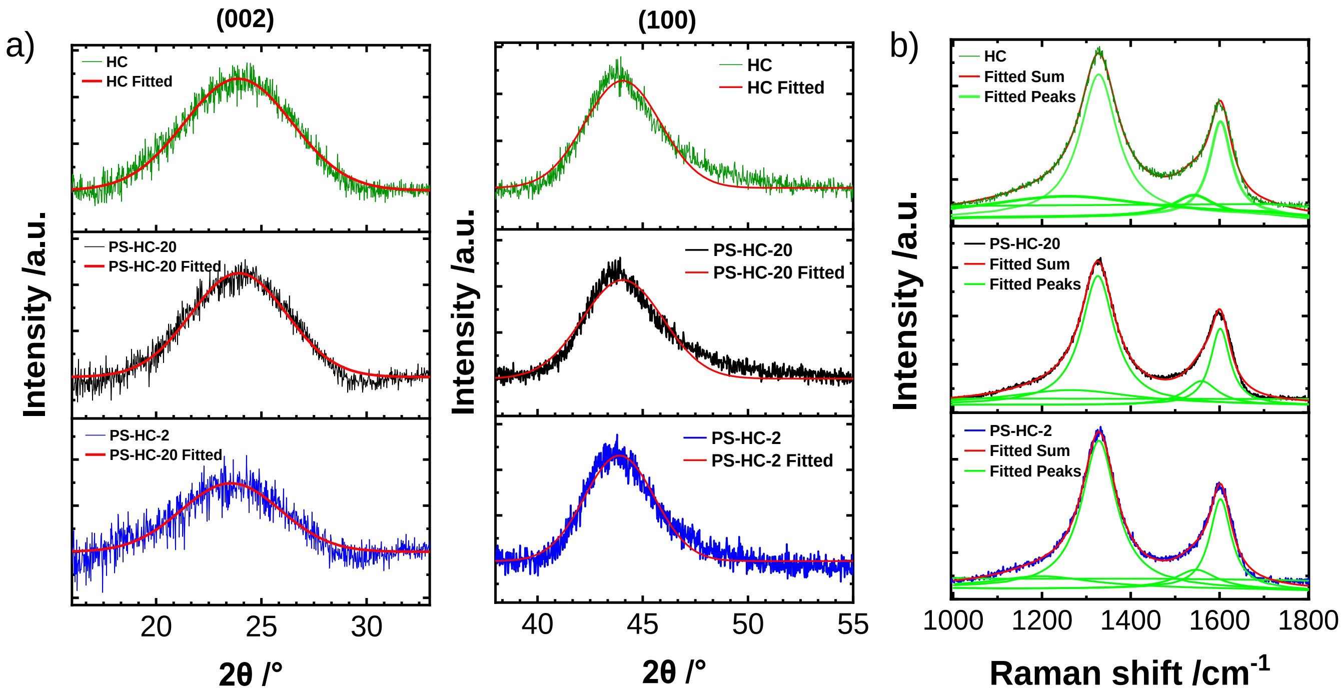

Figure S2. Fitted a) (002) and (100) reflections from powder X-Ray diffraction (PXRD) patterns. b) Raman spectra of hard carbon materials.

Table S2. Relevant characteristics of a hard carbon crystallite calculated from Scherrer equation.

	The crystalline coherency length in the stacking direction (L_c), nm	**The size of the layer in the plane direction (L_a), nm**
PS-HC-2	1.43	2.25
PS-HC-20	1.45	2.04
HC	1.36	2.08

Table S3. Intensity ratios of A- and G-band from Raman spectroscopy of hard carbon materials.

	I_A/I_G		I_A/I_G		I_A/I_G
PS-HC-2	0.22	**PS-HC-20**	0.32	**HC**	0.22

Table S4. Data obtained from physisorption isotherms (N_2 at 77 K and CO_2 at 273 K) of hard carbon materials: QSDFT, N_2 specific surface area and N_2 uptake, 2D-NLDFT, CO_2 pore volume, as well as CO_2 uptake.

	SSA_{QSDFT,N_2}, $m^2\,g^{-1}$	N_2 uptake at 77 K, $cm^3\,g^{-1}$	CO_2 uptake at 273 K, $cm^3\,g^{-1}$	$V_{CO_2(<0.7\ nm)}$, $cm^3\,g^{-1}$
PS-HC-2	10	15.1	3.8	0.010
PS-HC-20	1	2.1	0.4	0.003
HC	1	2.0	0.3	0.002

Table S5. Eemental analysis data of hard carbon materials.

	C, wt %	O, wt %	H, wt %
PS-HC-2	99.18	0.82	0
PS-HC-20	100.00	0	0
HC	99.93	0.07	0

Table S6. Values of H_2O uptake at 298 K of hard carbon materials.

	H_2O uptake at 298 K, $cm^3\,g^{-1}$		H_2O uptake at 298 K, $cm^3\,g^{-1}$		H_2O uptake at 298 K, $cm^3\,g^{-1}$
PS-HC-2	25.3	**PS-HC-20**	9.0	**HC**	12.1

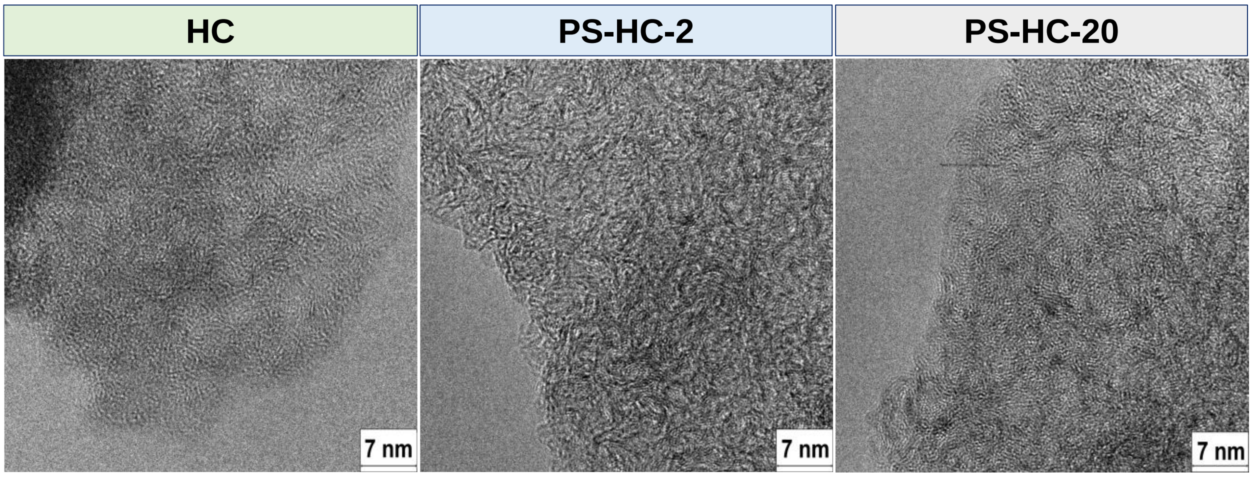

Figure S3. TEM images of hard carbon materials.

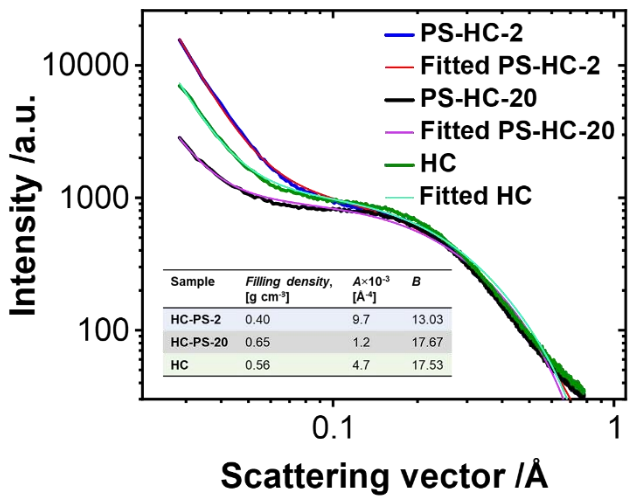

Figure S4. Fitted small-angle X-ray scattering (SAXS) curves of hard carbon materials.

Table S7. Pore characteristics of the materials determined from N_2 at 77 K and CO_2 at 273 K physisorptions of intermediate carbons after 600°C.

	$SSA_{QSDFT,N2}$, $m^2\ g^{-1}$	**V_{N2}, $cm^3\ g^{-1}$**	**$V_{CO2(<0.7\ nm)}$, $cm^3\ g^{-1}$**
PS-HC-2-600	566	0.22	0.174
PS-HC-20-600	464	0.20	0.181
HC-600	474	0.18	0.173

Table S8. Elemental analysis data of intermediate carbons after 600°C.

	C, wt %	**O, wt %**	**H, wt %**
PS-HC-2-600	90.79	6.67	2.54
PS-HC-20-600	90.95	6.75	2.30
HC-600	90.78	6.91	2.31

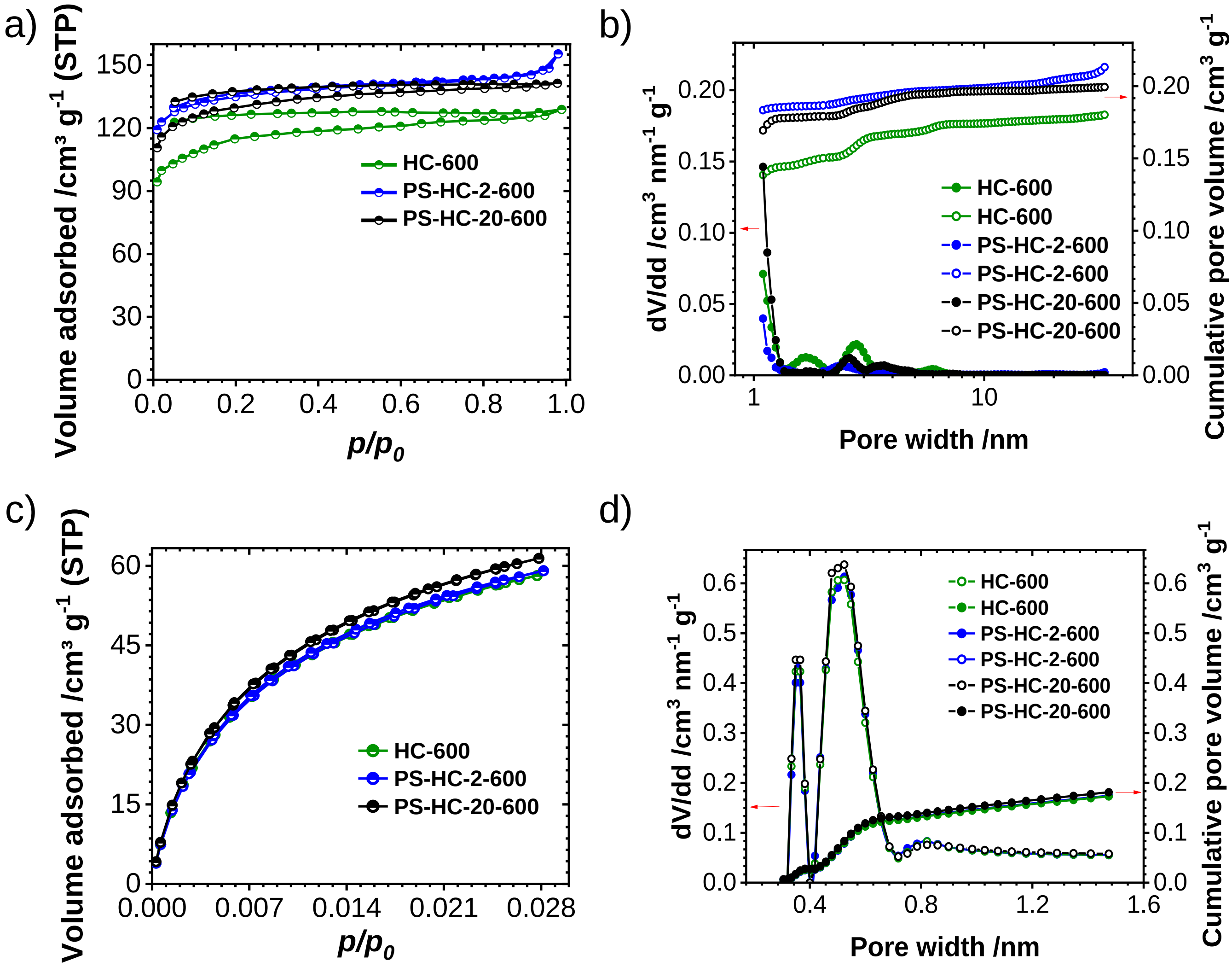

Figure S5. a) N_2-physisorption isotherms at 77 K; c) CO_2-physisorption isotherms at 273 K; b), d) Calculated pore size distributions of intermediate carbons after 600°C.

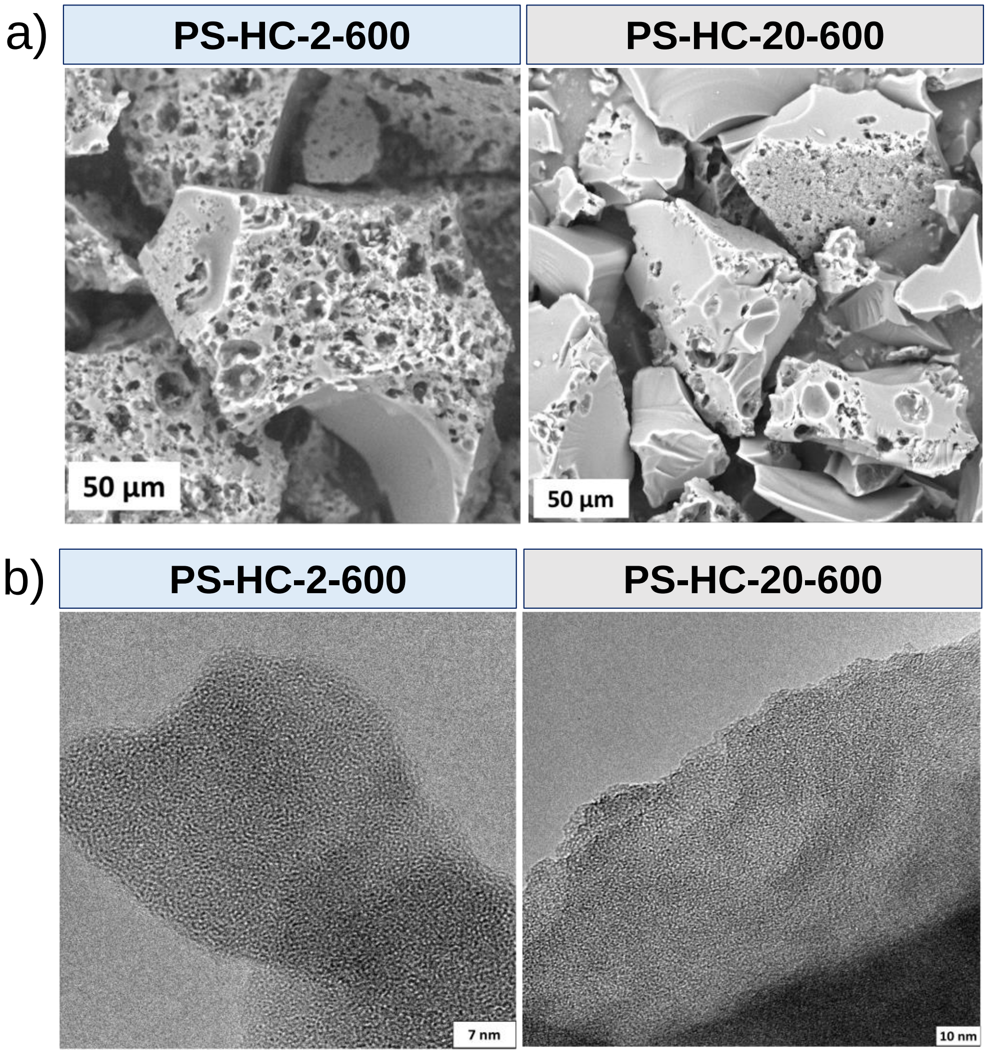

Figure S6. a) SEM images. b) TEM images of intermediate carbons after 600 °C.

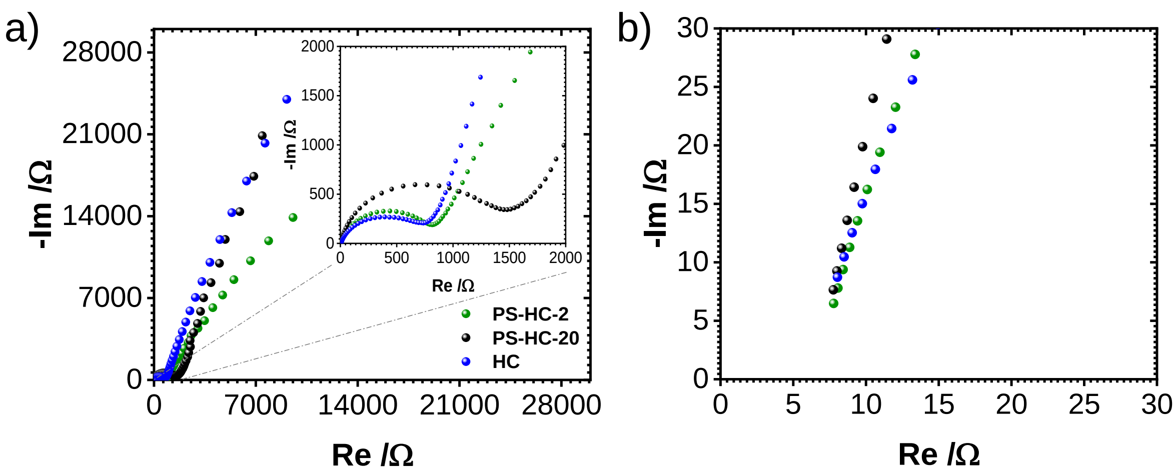

Figure S7. Electrochemical impedance spectra of hard carbons unaltered by solid electrolyte interphase (SEI).

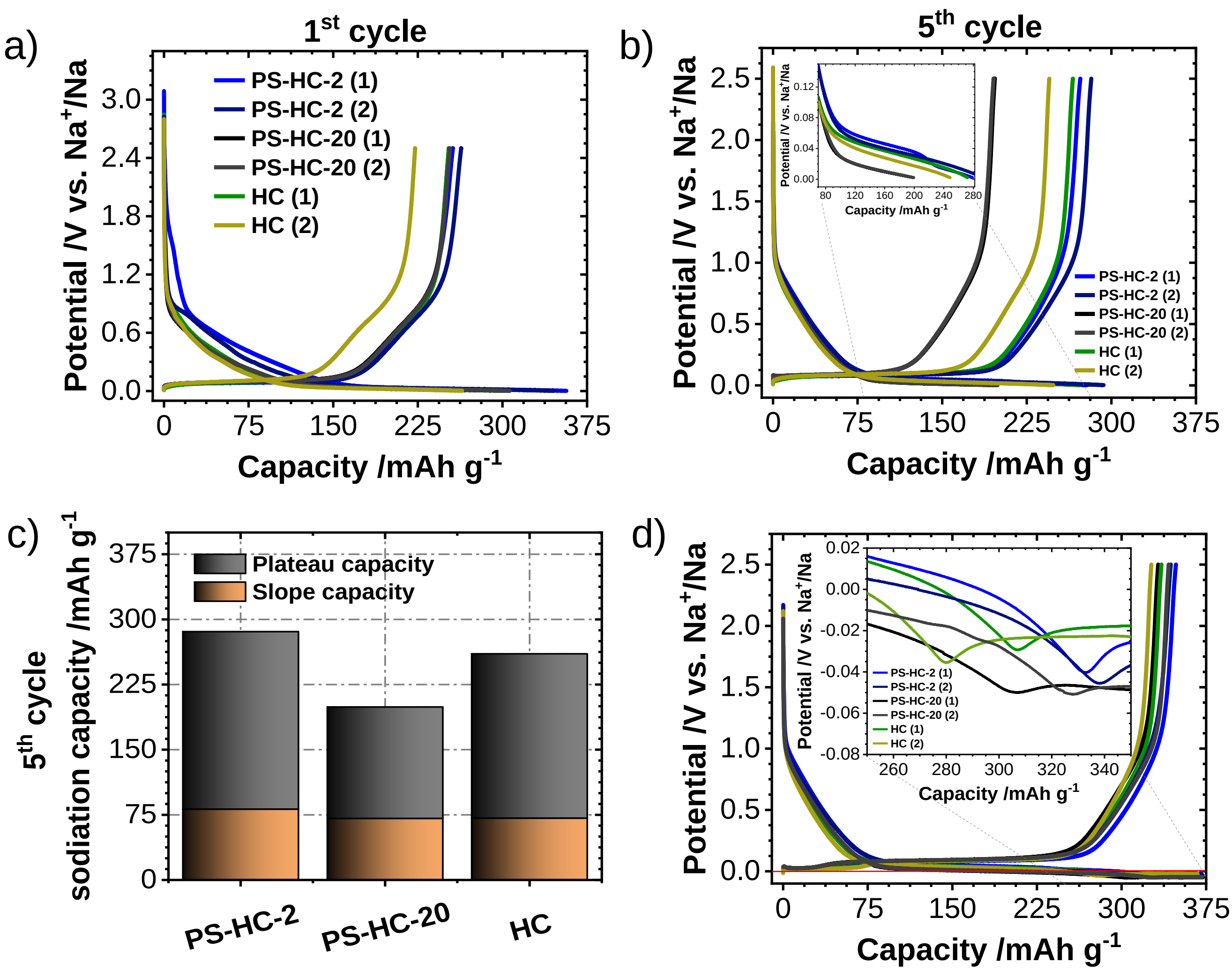

Figure S8. Galvanostatic charge-discharge curves of hard carbon materials recorded at C/20 current density from 2 experiments. a) Voltage limited 1st cycle. b) Voltage limited stable cycle (5th). c) A bar representing average from 2 experiments slope as well as plateau capacities of hard carbon materials in voltage limited stable cycle (5th). d) Capacity limited cycle.

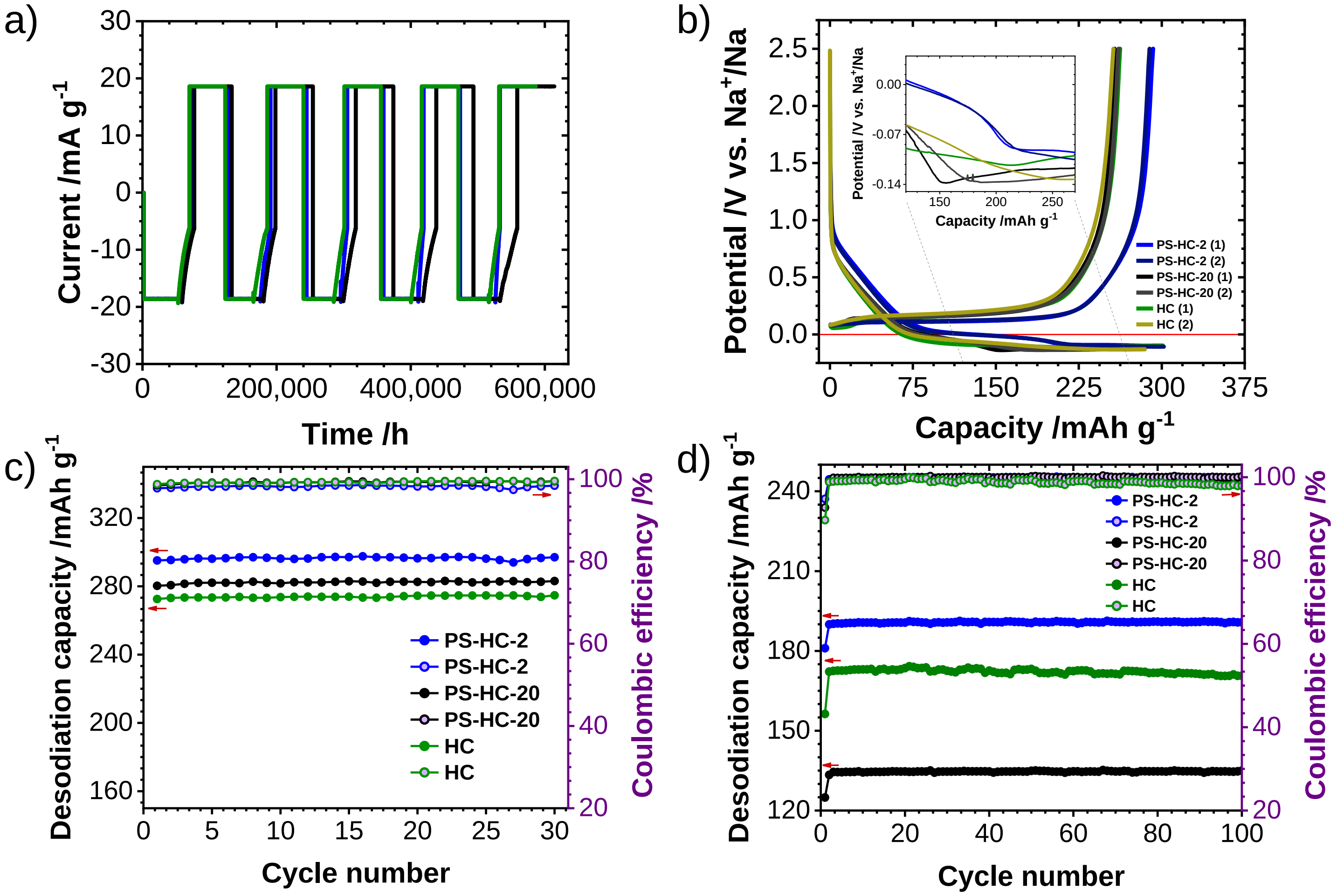

Figure S9. a) Representation in the scale current vs time of overall galvanostatic charge-discharge processes at C/20 current density with constant voltage step (2 mV). b) Capacity limited cycle of 2 experiments recorded at C/2 current density. c) Cycling at C/20 current density until 30 cycles with a capacity limitation. d) Cycling at C/2 current density until 100 cycles with a capacity limitation.