Electronic Supplementary Material (ESI) for Green Chemistry.

SUPPLEMENTARY INFORMATION

Addressing the energy sustainability of biowaste-derived hard carbon materials for battery electrodes

Arianna Baldinelli[1], Xinwei Dou[2,3], Daniel Buchholz[2,3], Mario Marinaro[4], Stefano Passerini[2,3,*], and Linda Barelli[1,*]

1- Department of Engineering – Università degli Studi di Perugia, via G. Duranti 93, 06125, Perugia, Italy

2- Helmholtz Institute Ulm (HIU), Helmholtzstraße 11, 89081, Ulm, Germany

3- Karlsruhe Institute of Technology (KIT), P.O. Box 3640, 76021, Karlsruhe, Germany

4- ZSW, Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, Helmholtzstr. 8, D-89081, Ulm, Germany

Corresponding authors: linda.barelli@unipg.it; stefano.passerini@kit.edu

SI 1 – Electrode cycling results

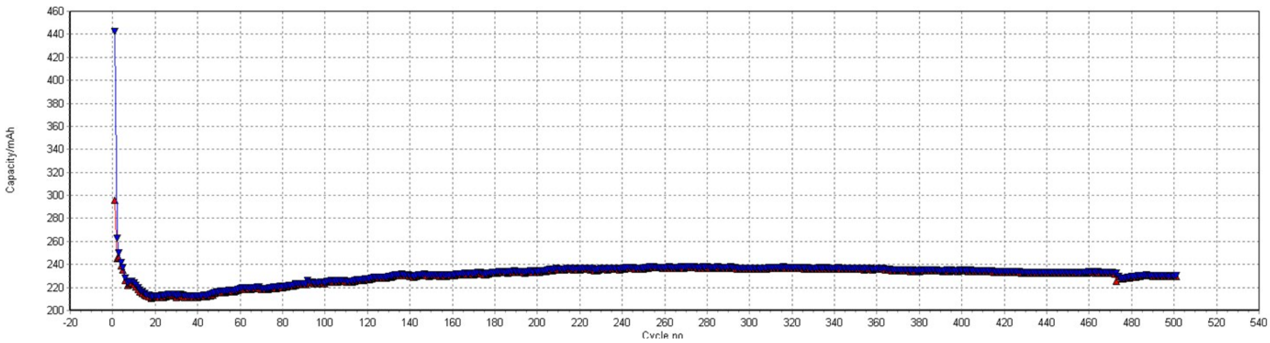

Figure SI-1. Long-term cycling performance of an apple pomace-derived hard carbon electrode in the Na//Hard carbon cell. Electrolyte: 1M $NaClO_4$ in EC: PC (1:1 wt.%). Charge and discharge current density: 200 mAh g^{-1}. For further details, please, see reference X. Dou, D. Buchholz, S. Passerini in APL Materials **6** (2018) 047501.

SI 2 - Extended model

Hereinafter detailed modelling equations are shown. In the main manuscript a condensed version of the equations is provided, in order to introduce theoretical elements which are accounted for. Yet, the main manuscript do not go to computational details. Moreover, a complete list of symbols adopted in the equations is attached to the Supplementary Information for the sake of clarity.

$$\sum_{j=1}^{3} x_j = x_{cell} + x_{hemi} + x_{lign} = 1$$ Eq. SI - 1

$$w_{subs}(T) = \sum_{j=1}^{3} x_j w_j(T) = x_{cell}\, w_{cell}(T) + x_{hemi}\, w_{hemi}(T) + x_{lign}\, w_{lign}(T)$$ Eq. SI - 2

$$\dot{h}_{subs}(T) = \sum_{j=1}^{3} x_j w_j(T) \dot{h}_j(T) = x_{cell} w_{cell}(T)\, \dot{h}_{cell}(T) + x_{hemi} w_{hemi}(T)\, \dot{h}_{hemi}(T) + x_{lign} w_{lign}($$ Eq. SI - 3

$$\dot{n}_{vi,subs}(T) = \sum_{j=1}^{3} x_j \dot{n}_{vi,\,j}(T) = x_{cell}\, \dot{n}_{vi,\,cell}(T) + x_{hemi}\, \dot{n}_{vi,\,hemi}(T) + x_{lign}\, \dot{n}_{vi,\,lign}(T)$$ Eq. SI - 4

$$\dot{m}_{i,subs}(T) = \frac{\dot{n}_{vi,subs}(T)\; PM_i}{V_{m,std}}$$ Eq. SI - 5

$$h_{subs}\big|_{A-B} = \int_{ta}^{tb} \dot{h}_{subs}(T)\, dt = \int_{Ta}^{Tb} \dot{h}_{subs}(T)\, \frac{dT}{TR}$$ Eq. SI - 6

$$H_{subs}\big|_{A-B} = m_{subs}\, h_{subs}\big|_{A-B}$$ Eq. SI - 7

$$h_{comb}\big|_{K-J} = \int_{tk}^{tj} \sum_{i=1}^{l} \dot{m}_i(T)\; LHV_i\, dt = \int_{Tk}^{Tj} \sum_{i=1}^{l} \dot{m}_i(T)\; LHV_i\, \frac{dT}{TR'}$$ Eq. SI - 8

$$(m_{hc} + m_{lbs} + m_{tar}) + m_{pyrogas} = (m_{hc} + m_{lbs} + m_{tar}) + \sum_{i=1}^{l} \int_{RT}^{Tfin} \dot{m}_i(T)\, \frac{dT}{TR'} = 1$$ Eq. SI - 9

$$h_{subs}\big|_{K-J} = \varphi \Delta H_{wat,(RT-T_{ev})} + (1-\varphi)\Delta H_{subs,(RT-T_{pyr})}$$ Eq. SI - 10

$$\Delta H_{wat,\left(RT-T_{ev}\right)} = \bar{c}_{wat}\left(T_{ev} - RT\right) + \Delta H_{ev,wat}\left(T_{ev}\right)$$ Eq. SI - 10a

$$\Delta H_{subs,\left(RT-T_{pyr}\right)} = \bar{c}_{p,subs}(T)\left(T_{pyr} - RT\right) + \int_{Tpyr}^{Tfin} \dot{h}_{subs}(T)\, \frac{dT}{TR}$$ Eq. SI - 10b

$$\eta_{pyr} = \frac{m_{pyrogas} L\bar{H}V_{pyrogas} + \tilde{m}_{tars} L\bar{H}V_{tars} + m_{hc} L\bar{H}}{m_{subs}\left[\left(\sum_{j=1}^{3} x_j LHV_j\right) + \left|DH_{pyr}\right|\right]}$$ Eq. SI - 11

List of Symbols and abbreviations

Symbols

$\dot{h}$	[W g^{-1}]	reaction specific heat release/uptake rate
h	[J g^{-1}]	reaction specific heat release/uptake
i	-	fibres components index (from 1 to 3)
j	-	volatile gases components index (from 1 to 6)
H	[J]	reaction total heat release/uptake
LHV	[MJ kg^{-1}]	Low Heating Value
$\dot{m}$	[g min^{-1}]	mass flow rate (absolute or specific to substrate initial mass)
m	[g],[kg]	mass (absolute or specific to substrate initial mass)
$\dot{n}_v$	[ml min^{-1}]	volume flowrate (absolute or specific to substrate initial mass)
PM	[g mol^{-1}]	molecular weight
t	[s], [min]	time
T	[°C]	temperature
TR	[°C min^{-1}]	temperature rate
V_m	[l mol^{-1}]	molar volume
w	[%]	residual mass (as a fraction of the original specimen mass)
x	[%]	mass fraction

Subscripts

as	as received
cell	cellulose
comb	combustion
hemi	hemicellulose
lbs	low boiling substances (including water)
lign	lignin
std	standard
subs	substrate
wat	water