# ChemSusChem

Supporting Information

## Performance and Sustainability Tradeoffs of Oxidized Carbon Nanotubes as a Cathodic Material in Lithium-Oxygen Batteries

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#### **Figures**

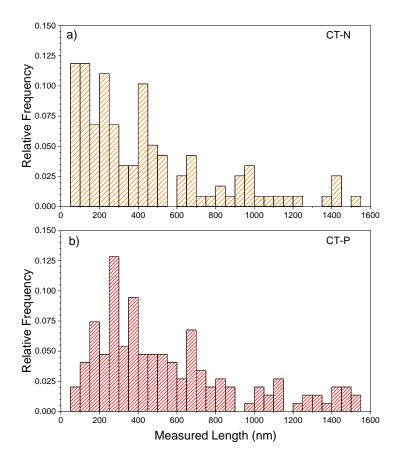


Figure S1: Length distribution of a) nitric acid-treated MWCNTs and b) pristine MWCNTs, as determined by scanning electron microscopy imaging.

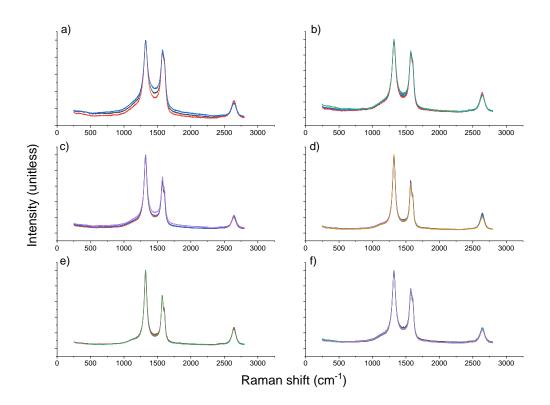


Figure S2: Raman spectra for all MWCNT samples used in this study: a) CT-P, b) CT-P-900, c) CT-N, d) CT-N-400, e) CT-N-600, f) CT-O. The G-band is at ~1575 cm<sup>-1</sup> and the D-band is at ~1325 cm<sup>-1</sup>.

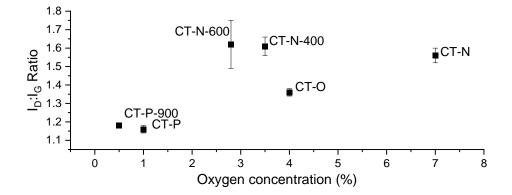


Figure S3: The relationship between disorder and surface chemistry, in the form of  $I_D:I_G$  ratio vs. percent total surface oxygen for samples of different surface chemistry.

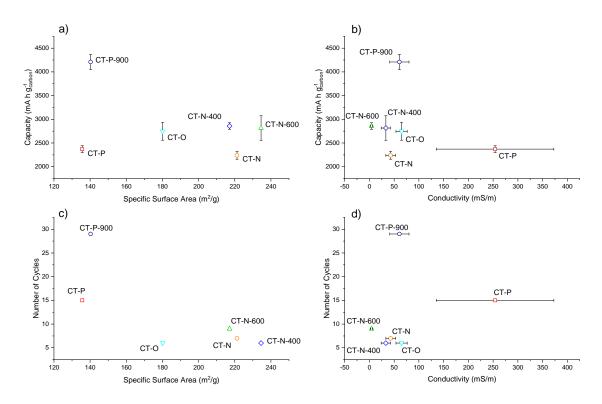


Figure S4: The relationship between capacity and a) specific surface area of MWCNT powder and b) conductivity of MWCNT:PVDF cathode, and the relationship between the number of completed cycles and c) specific surface area of MWCNT powder and d) conductivity of MWCNT:PVDF cathode.

### Life Cycle Assessment Inventory:

Fluidized Bed Chemical Vapor Deposition (1 g MWCNT)

Heating	Flow	Provider	Amount	Unit
	argon, liquid	market for argon, liquid   argon, liquid   Cutoff, U – RoW	216.92	g
	electricity, low voltage	market group for electricity, low voltage   electricity, low voltage   Cutoff, U – US	0.18	kWh
Catalyst Deposition	Flow	Provider	Amount	Unit
	aluminium oxide, metallurgical	market for aluminium oxide, metallurgical   aluminium oxide, metallurgical   Cutoff, U – RoW	153.85	g
	Aluminum isopropoxide	Stoichiometrically estimated	0.05	g
	argon, liquid	market for argon, liquid   argon, liquid   Cutoff, U – RoW	133.08	g
	oxygen, liquid	market for oxygen, liquid   oxygen, liquid   Cutoff, U – RoW	4.38	g
	Ferrocene	Stoichiometrically estimated	0.02	g
	electricity, low voltage	market group for electricity, low voltage   electricity, low voltage   Cutoff, U – US	0.04	kWh
Annealing	Flow	Provider	Amount	Unit
	argon, liquid	market for argon, liquid   argon, liquid   Cutoff, U – RoW	160.48	g
	electricity, low voltage	market group for electricity, low voltage   electricity, low voltage   Cutoff, U – US	0.07	kWh
	hydrogen, gaseous	market for hydrogen, gaseous   hydrogen, gaseous   Cutoff, U – GLO	2.82	g
	water, deionised	market for water, deionised   water, deionised   Cutoff, U – RoW	0.06	g
MWCNT Growth	Flow	Provider	Amount	Unit
	acetylene	market for acetylene   acetylene   Cutoff, U – RoW	1.55	g
	argon, liquid	market for argon, liquid   argon, liquid   Cutoff, U – RoW	158.08	g
	hydrogen, gaseous	market for hydrogen, gaseous   hydrogen, gaseous   Cutoff, U – GLO	2.82	g
	water, deionised	water production, deionised   water, deionised   Cutoff, U – RoW	0.06	g
	water, actornated			

Separation

Flow

market for argon, liquid   argon, liquid			
argon, liquid	Cutoff, U – RoW	68.85	g
electricity, low voltage	market group for electricity, low voltage   electricity, low voltage   Cutoff, U – US	0.01	kWh
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#### Hot Wall Chemical Vapor Deposition

Catalytic Particle Production (10 g)	— Flow	Provider	Amount	Unit
	electricity, low	market group for electricity, low voltage		
	voltage	electricity, low voltage   Cutoff, U - US	0.9	kWh
		market for iron (III) chloride, without		
	iron (III) chloride,	water, in 40% solution state   iron (III)		
	without water, in	chloride, without water, in 40% solution	54.40	~
	40% solution state	state   Cutoff, U – GLO	54.12	g
		market for nitrogen, liquid   nitrogen,		
	nitrogen, liquid	liquid   Cutoff, U – RoW	126	g
		market for water, deionised   water,		
	water, deionised	deionised   Cutoff, U – RoW	100	g
		market for zeolite, powder   zeolite,		
	zeolite, powder	powder   Cutoff, U – GLO	10	g
MWCNT Growth (7.5 g)	Flow	Provider	Amount	Unit
		market for acetylene   acetylene   Cutoff,		
	acetylene	U – RoW	18.4	g
	Catalytic Particles	Calculated above	0.22	g
	electricity, low	market group for electricity, low voltage		
	voltage	electricity, low voltage   Cutoff, U – US	2.3	kWh
		market for nitrogen, liquid   nitrogen,		
	nitrogen, liquid	liquid   Cutoff, U – RoW	160.8	g

#### **Nitric Acid** Treatment (8 g MWCNT) Provider Flow Amount Unit market group for electricity, low voltage | electricity, low voltage | Cutoff, U – US electricity, low voltage 560 Wh market for nitric acid, without water, in 50% nitric acid, without water, in 50% solution solution state | nitric acid, without water, in state 50% solution state | Cutoff, U – RoW 284 g

Ozonation (2 g MWCNT)	Flow	Provider	Amount	Unit
	-	market group for electricity, low voltage		
	electricity, low voltage	electricity, low voltage   Cutoff, U – US	105	Wh
	oxygen, liquid	market for oxygen, liquid   oxygen, liquid   Cutoff, U – RoW	10	g
	water, deionised	water production, deionised   water, deionised   Cutoff, U – RoW	20	g

High Temperature Annealing (2 g MWCNT)	_			
400°C	Flow	Provider	Amount	Unit
	electricity, low voltage	market group for electricity, low voltage   electricity, low voltage   Cutoff, U – US	0.186	kWh
	helium	market for helium   helium   Cutoff, U – GLO	7.854	g
600°C	Flow	Provider	Amount	Unit
	electricity, low voltage	market group for electricity, low voltage   electricity, low voltage   Cutoff, U – US	0.2755	kWh
	helium	market for helium   helium   Cutoff, U – GLO	9.996	g
900°C	Flow	Provider	Amount	Unit
	electricity, low voltage	market group for electricity, low voltage   electricity, low voltage   Cutoff, U – US	0.6422	kWh
	helium	market for helium   helium   Cutoff, U – GLO	11.781	g