Supplementary Materials

Dual-Template Ordered Mesoporous Carbon/Fe_2O_3 Nanowires as Lithium-ion Battery Anodes

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1. Calculations

The absolute (ΔV_{meso}) and relative (ΔV_{meso} %) mesoporous volume difference between OMC/Fe_2O_3 composites and their corresponding OMCs were calculated through the following equations:

$$\Delta V_{meso} = V_{meso-C} - V_{meso-CFe} / (1 - Fe_2O_3\ wt\%) \quad \text{(S1)}$$

$$\Delta V_{meso}\% = \frac{\Delta V_{meso}}{V_{meso-C}} \times 100 \quad \text{(S2)}$$

Here, $V_{meso\text{-}CFe}$ and $V_{meso\text{-}C}$ are mesopore volume of OMC/Fe_2O_3 composites and mesopore volume of pure OMCs; Fe_2O_3 *wt%* is the mass percentage of Fe_2O_3 in the OMC/Fe_2O_3 composites; $V_{meso-CFe} / (1 - Fe_2O_3\ wt\%)$ is the mesopore volume of OMC/Fe_2O_3 composites normalized by the initial carbon mass.

2. Figures and Tables

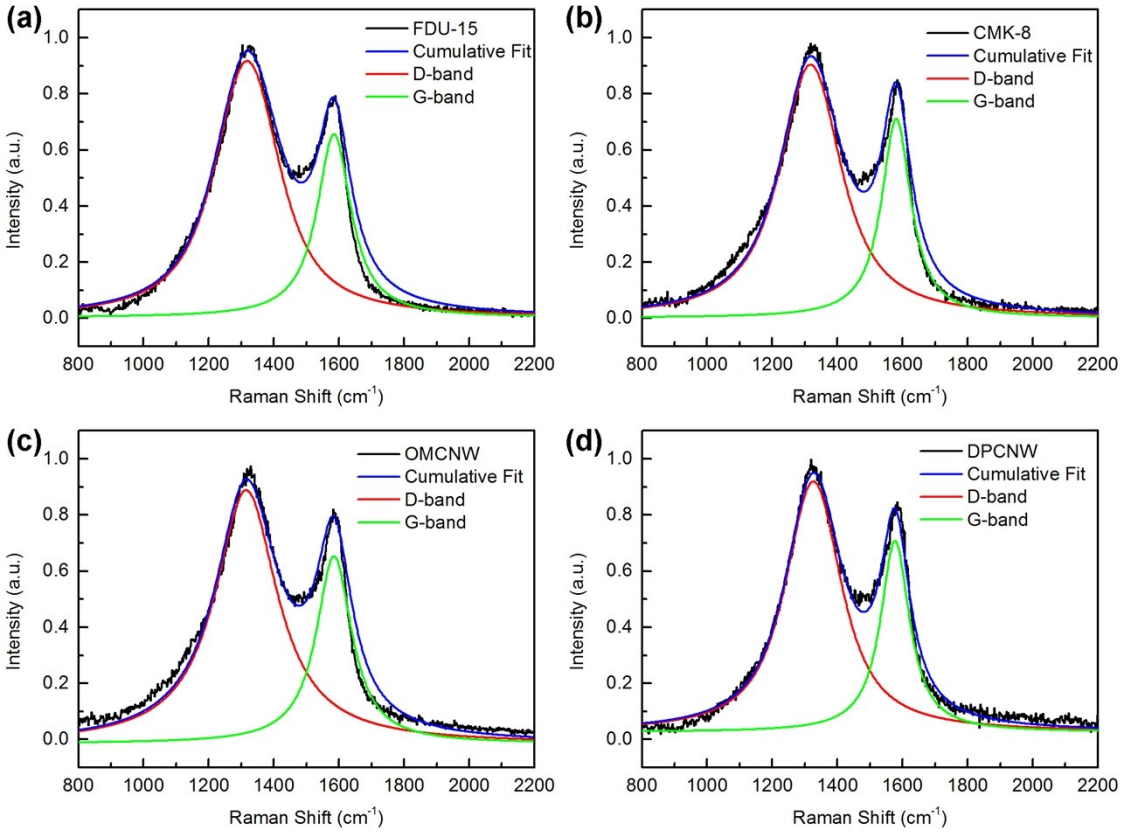

Figure S1. De-convoluted Raman D and G bands of (a) FDU-15, (b) CMK-8, (c) OMCNW, and (d) DPCNW.

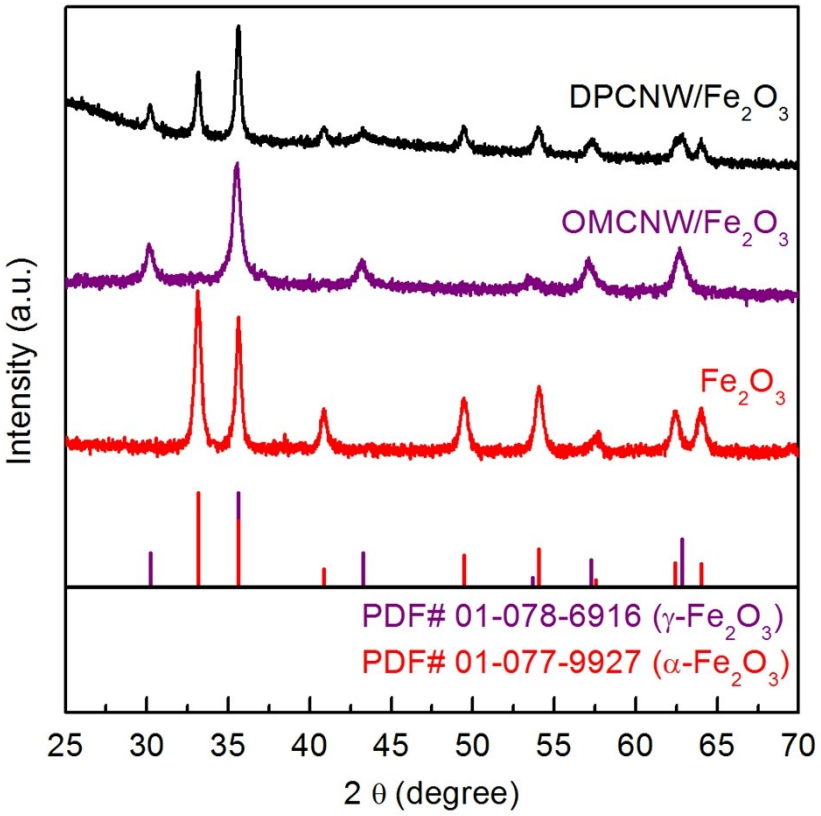

Figure S2. XRD spectra of OMCNW/Fe_2O_3, DPCNW/Fe_2O_3, and Fe_2O_3. The standard peaks of γ-Fe_2O_3 and α-Fe_2O_3 are given in the bottom panel. The Fe_2O_3 sample is synthesized by directly annealing $Fe(NO_3)_3 \cdot 9H_2O$ without adding any carbon materials. The anneal process is the same as that for OMC/Fe_2O_3.

The carbon-free Fe_2O_3 shows a pure alpha phase, indicating the decomposed product of $Fe(NO_3)_3 \cdot 9H_2O$ is α-Fe_2O_3. However, it is known in the literature that the alpha phase transforms to gamma phase when carbon is introduced into the system, which is very likely due to the interaction of carbon with $Fe(NO_3)_3$ during the decomposition process.[1-4] The Fe_2O_3 in OMCNW/Fe_2O_3 and other OMC/Fe_2O_3 composites in this work are γ-Fe_2O_3. In the case of DPCNW/Fe_2O_3, the outer surface of Fe_2O_3 particles are in contact with carbon and formed γ-Fe_2O_3 on the outer surface, whereas the inner parts of Fe_2O_3 particles do not directly interact with carbon due to the large particle size. Therefore, the Fe_2O_3 particles inside of DPCNW show mixed phases of α-Fe_2O_3 and γ-Fe_2O_3.

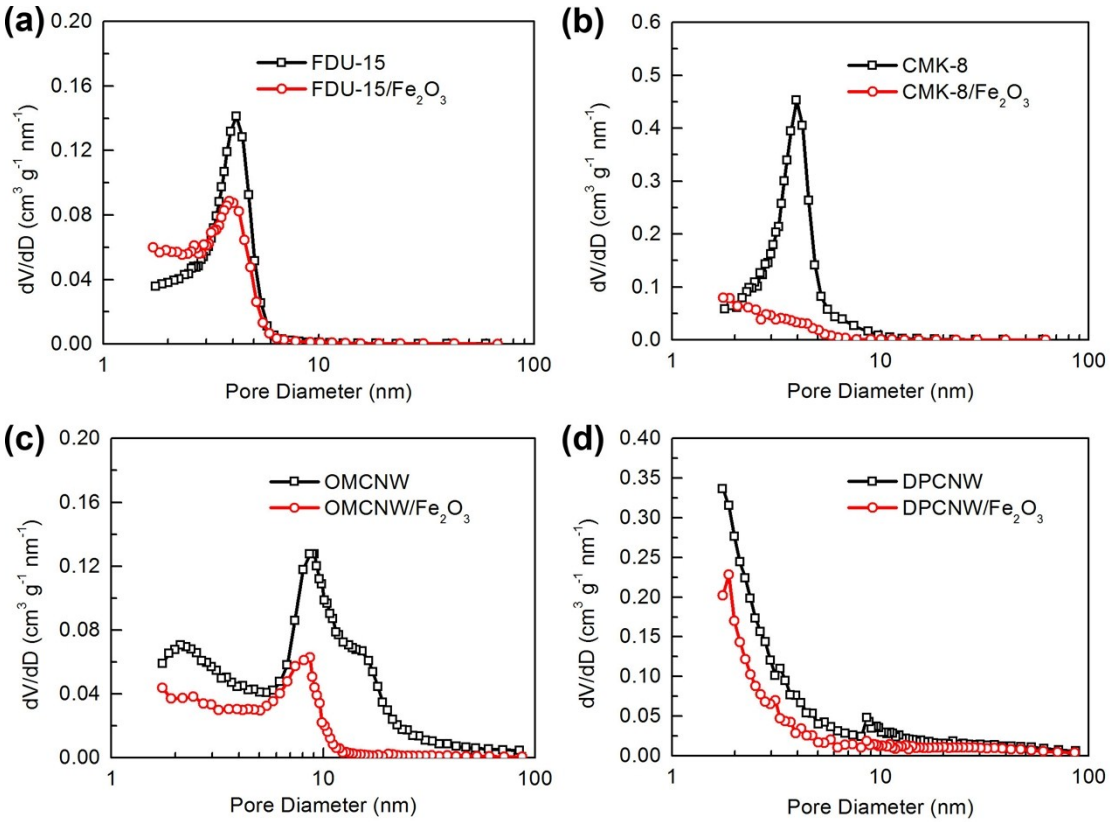

Figure S3. Pore size distributions of porous carbons and carbon/Fe_2O_3 composites.

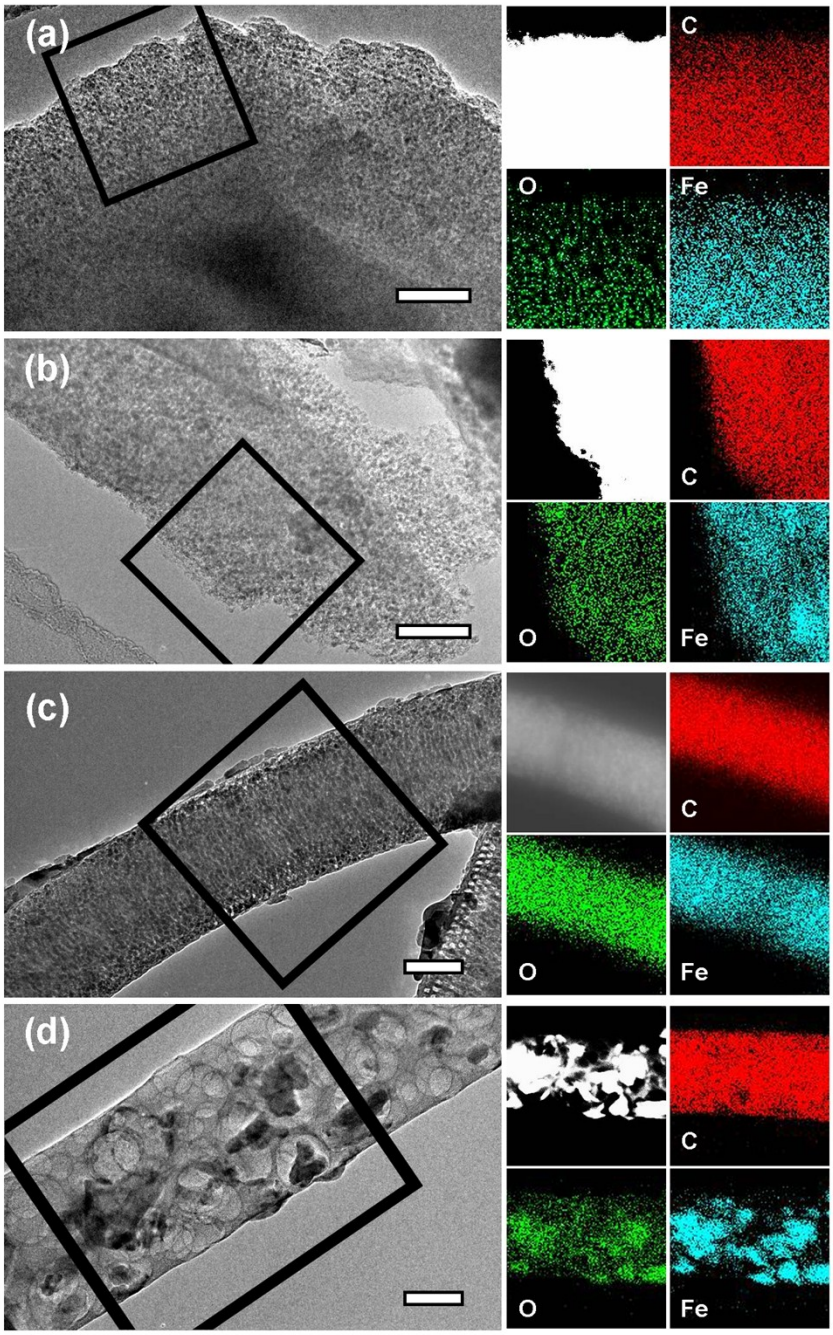

Figure S4. TEM images (left) and EDX mappings (right) of (a) FDU-15/Fe_2O_3, (b) CMK-8/Fe_2O_3, (c) OMCNW/Fe_2O_3, and (d) DPCNW/Fe_2O_3. All scale bars in the TEM images are 100 nm. The black squares in TEM images are the spots where EDX were taken. The carbon, oxygen, and iron in EDX mappings were represented by red, green, and blue colors, respectively.

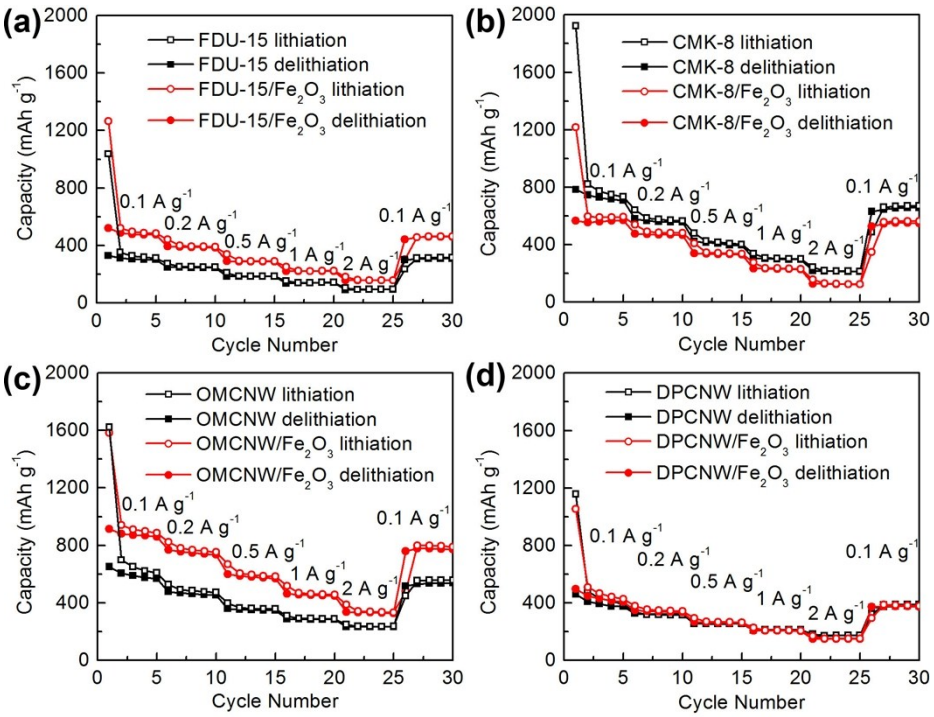

Figure S5. Comparison of rate performances of (a) FDU-15 and FDU-15/Fe_2O_3, (b) CMK-8 and CMK-8/Fe_2O_3, (c) OMCNW and OMCNW/Fe_2O_3, and (d) DPCNW and DPCNW/Fe_2O_3. Solid: lithiation; open: delithiation.

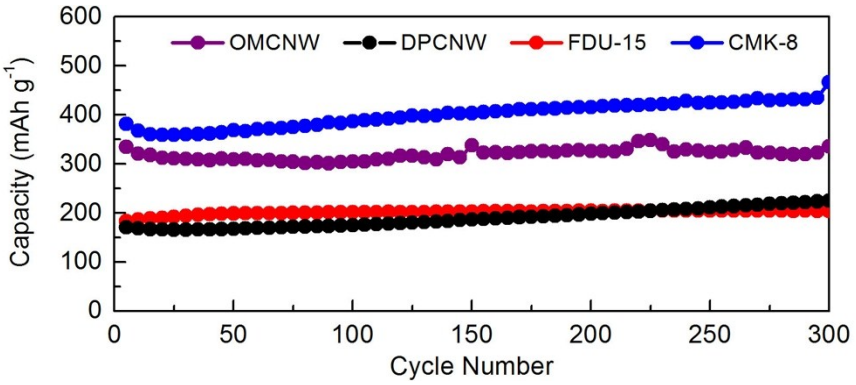

Figure S6. Electrochemical cycling performances of FDU-15, CMK-8, DPCNW, and OMCNW. The first 3 cycles are at 0.1 A g^{-1} for activation of electrodes (For clarity, data are not shown).

Table S1. EIS parameters for different carbon/Fe_2O_3 composites

Sample ID	R_s (Ω)	R_{SEI+ct} (Ω)	Z (Ω)
OMCNW/Fe_2O_3	3	64	18
FDU-15/Fe_2O_3	4	69	47
DPCNW/Fe_2O_3	3	139	31
CMK-8/Fe_2O_3	3	168	88

Table S2. Estimated volume changes during lithiation process in carbon/Fe_2O_3 composites.

Sample ID	V_{Fe2O3} ($cm^3\ g^{-1}$)	ΔV_{Fe2O3} ($cm^3\ g^{-1}$)	V_C ($cm^3\ g^{-1}$)	ΔV_C ($cm^3\ g^{-1}$)	ΔV_t ($cm^3\ g^{-1}$)	V_t ($cm^3\ g^{-1}$)	$\Delta V_t/V_t$
OMCNW/Fe_2O_3	0.0858	0.172	0.24	0.024	0.196	0.444	44 %
FDU-15/Fe_2O_3	0.0288	0.058	0.38	0.037	0.095	0.264	36 %
DPCNW/Fe_2O_3	0.0361	0.072	0.36	0.036	0.108	0.157	69 %
CMK-8/Fe_2O_3	0.0683	0.137	0.28	0.028	0.165	0.175	94 %

V_{Fe2O3}: Fe_2O_3 volume based on Fe_2O_3 density of 5.242 g cm^{-3};
V_C: carbon volume based on graphite density of 2.267 g cm^{-3};
ΔV_{Fe2O3}: Fe_2O_3 volume expansion estimated from 200 % Fe_2O_3 volume increase;[5]
ΔV_C: carbon volume expansion estimated from 10 % graphite volume increase;[6]
ΔV_t: total volume expansion from ΔV_{Fe2O3} and ΔV_C;
V_t: total volume from N_2 sorption-desorption;
$\Delta V_t/V_t$: ration between changed volume and total volume.

References

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4. N. Liu, J. Shen and D. Liu, *Electrochimica Acta*, 2013, **97**, 271-277.
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