A Novel Mesoporous Carbon-Silica-Titania Nanocomposite as High Performance Anode Material in Lithium Ion Batteries

Yuanyuan Zhou[a], Younghun Kim[a], Changsin Jo[b], Jinwoo Lee[b], Chul Wee Lee[a], Songhun Yoon*[a]

,

[a] *Green Chemical Technology Division, Korea Research Institute of Chemical Technology (KRICT) & University of Science and Technology (UST), Daejeon 305-600, Korea, E-mail: yoonshun@krict.re.kr*

[b] *Department of Chemical Engineering, Pohang University of Science and Technology, Kyungbuk 790-784, Korea*

Synthesis of m-CST and m-CT: The resol precursor (M_w < 500) was prepared similar to the literature method.[1] In a typical procedure, 0.61 g of melted phenol was mixed with 0.13 g of 20 wt % NaOH aqueous solution under stirring for 10 min. Then 1.05 g of formalin (37 wt % formaldehyde) was added dropwise below 50 °C. After stirring for 1h at 70-75 ^{o}C the mixture was cooled down to room temperature and the pH value was adjusted to about 7.0 using 0.1M HCl solution. Then water was removed by vacuum evaporation. Enough THF was added and filtration was done in order to remove the NaCl. Then, with THF removed, final product was acquired. Finally the final resol precursors were dissolved in ethanol (20 wt % ethanolic solution) for use. Titanium Citrate Complex was prepared using a simple and similar procedure from the literature method.[2] 0.1mol $Ti(OPr)_4$ (from Ardrich) was dissolved in 75ml ethanol while 0.1mol

Citrate acid (Ardrich) in 100ml ethanol. The citrate acid solution was added into the $Ti(OEt)_4$ solution dropwise under stirring. Upon further stirring at 40 ^oC for 2 hr in a closed flask, the total volumn of the solution was adjusted to 200 ml by adding ethanol. The final solution (0.5M Titanium Citrate Complex) was ready for direct experimental use. Similar to the reported tri-constituent co-assembly synthesis method for mesopous carbon, in a typical procedure, 1.6 g F127 and 1g 0.1 M HCl was added was added into 10g ethnol/H2O mixture(4:1).[1,3,4] The mixture was stirred at room temperature until a clear solution was acquired. Then 2.08 g TEOS and 5 g resol ethnolic solution were added and subsequently 4ml 0.5 M Titanium Citrate solution was dropped when the solution turned orange immediately. Upon stirring at room temperature for 2h, the orange clear solution was transferred to a big dish and kept in ambient environment for fully evaporation of ethanol and glue-like film was formed. Then the dish was transferred into an oven at 100 ^oC for polymerization. The polymerized film with dark color was obtained. After grinding, as-obtained powders were calcined in a tubular furnace at 450 ^oC for 2 hr and further calcined at 750 ^oC for 2 hr under N_2 flow. After cooling down to the room temperature, the sample named m-CST as was taken out and and its anode performance was investigated after fabrication of electrode. In order to selectively remove the embedded silica of m-SCT, a NaOH etching was tried. In this

procedure, the sample m-SCT was mixed with 15% NaOH aqueous solution. After stirring, the result powders were filtrated, washed for several time and dried. The final product was indexed as m-CT.

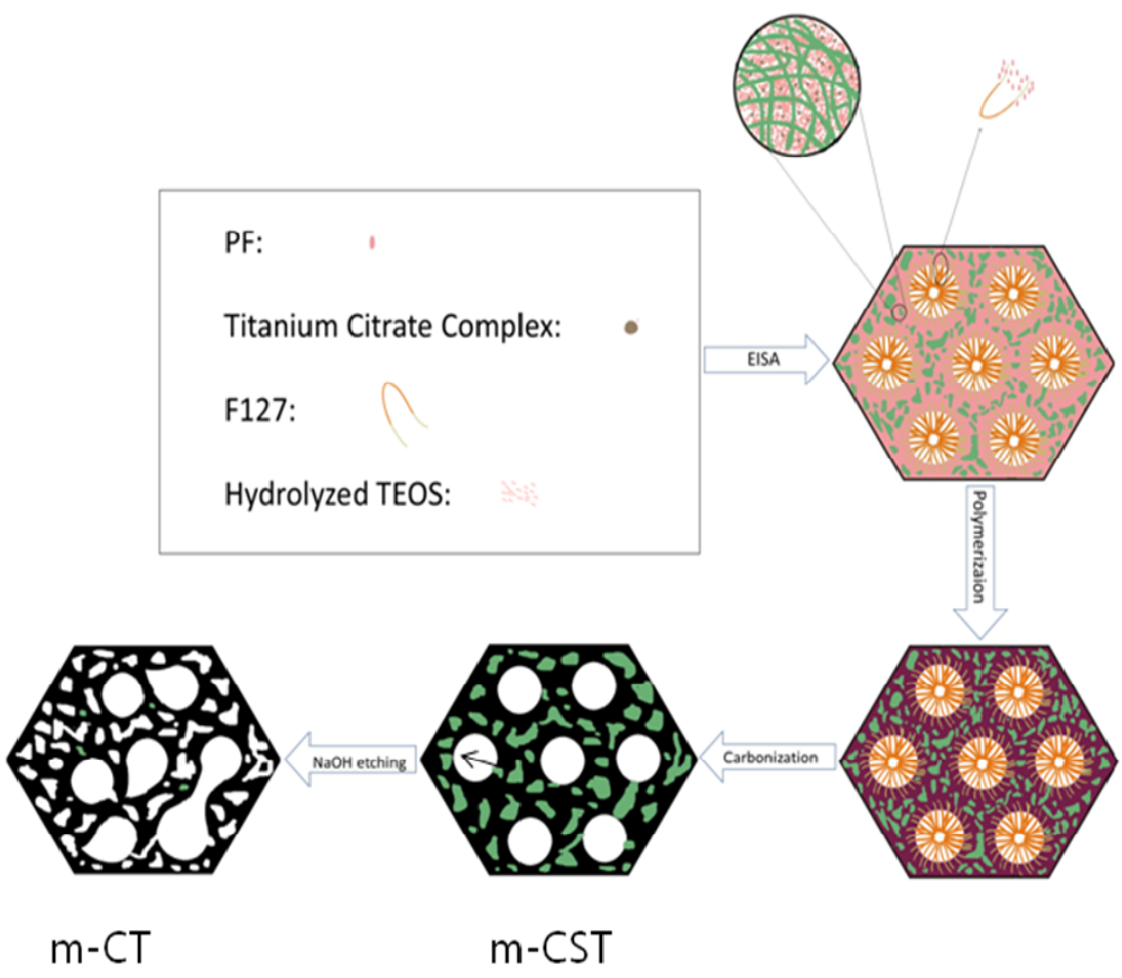

Figure S1. Schematic representation of synthesis of m-CST and m-CT using a tetra-constituents co-assembly method via. evaporation induced self-assembly process.

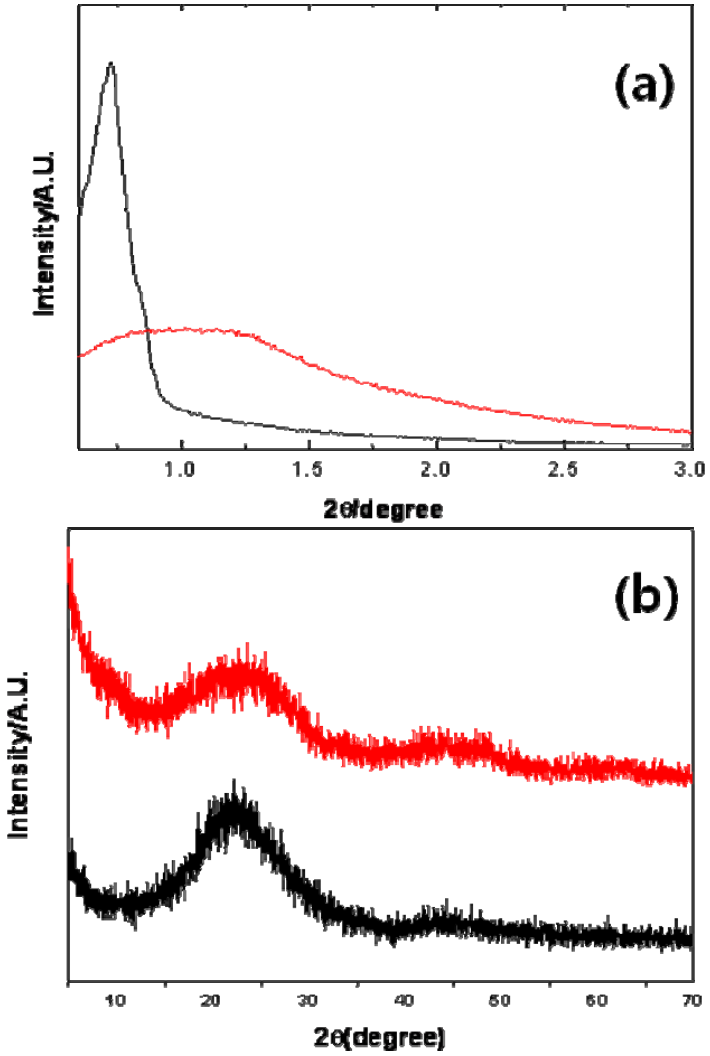

Figure S2. (a) Small angle x-ray diffraction patterns for m-CST (black line) and m-CT (red line) (b) Wide angle x-ray diffraction patterns for m-CST (black line) and m-CT (red line).

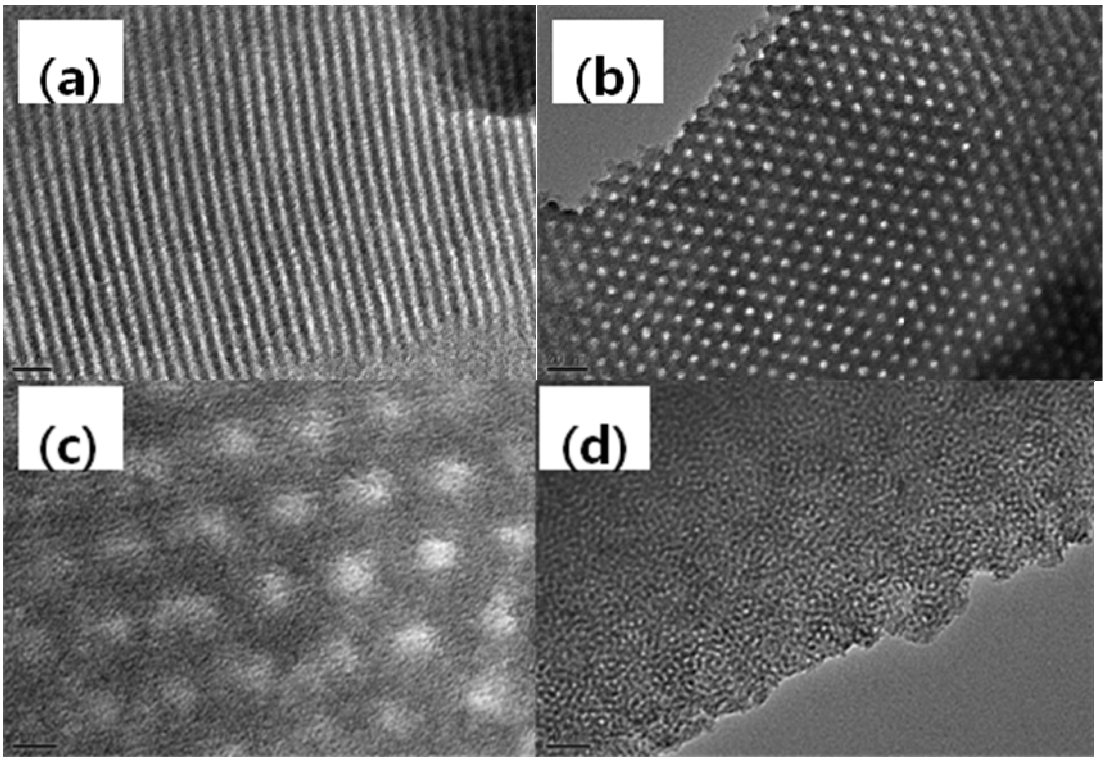

Figure S3. TEM images of m-CST showing a highly ordered hexagonal mesoporous structure from (a) to (c). In (c), a high resolution TEM (HRTEM) image was shown. As seen, no small sized crystal of TiO2 and SiO2 was observed. (d) TEM image of m-CT, which display a wormhole-like pore structure.

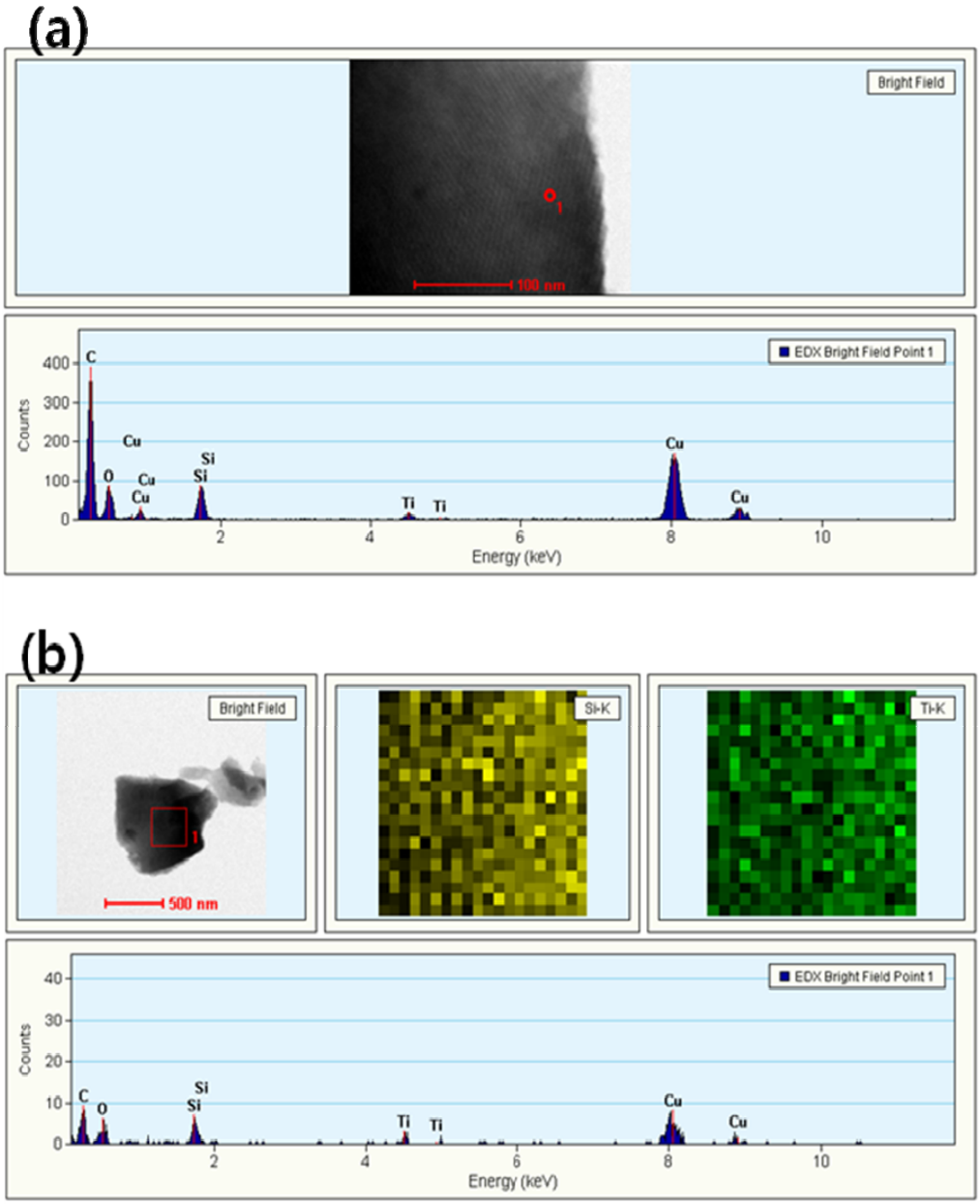

Figure S4. Energy dispersive x-ray spectroscopy from TEM experiment for m-CST (a) The elemental analysis for a point as red circle (b) The elemental analysis for a area as red rectangle. Clearly, carbon, Si and Ti are observed for both analysis.

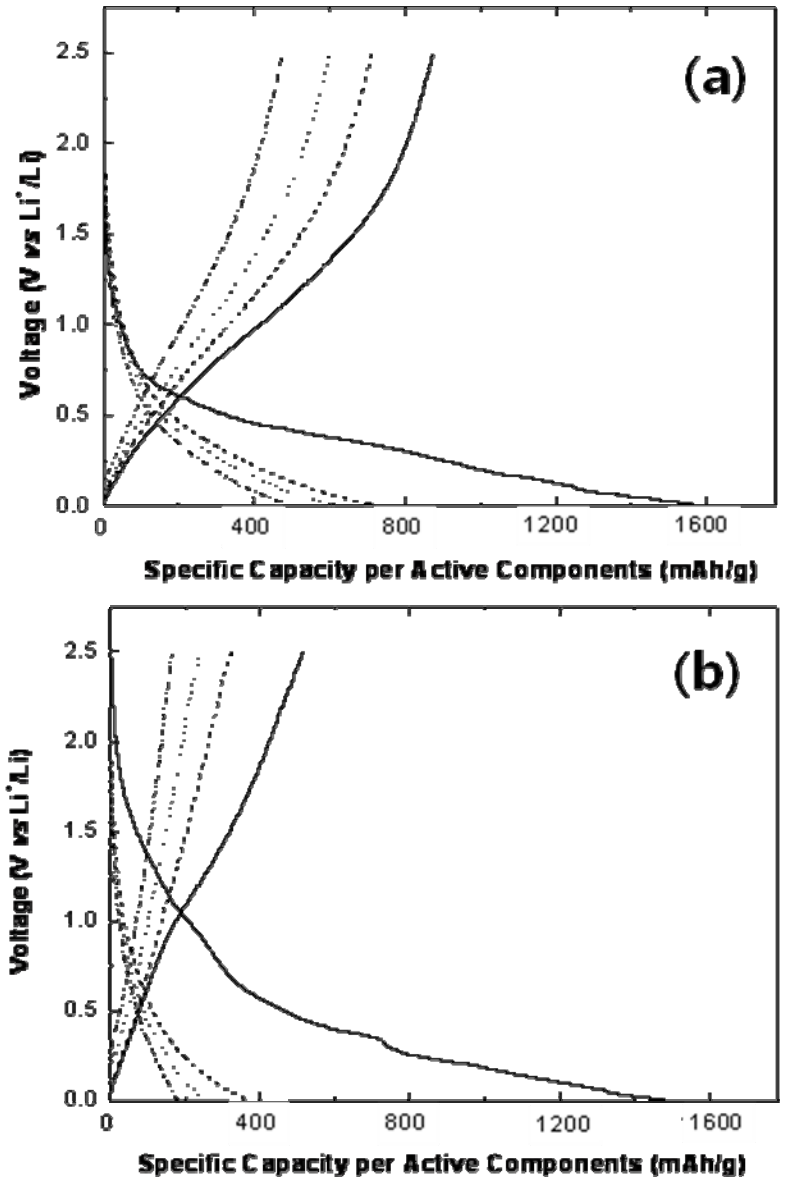

Figure S5. Galvanostatic charge-discharge patterns with change of applied current from 0.1 to 1 C rate for m-CST; (a), and m-CT; (b).

References

1 R. Liu, Y. Shi, Y. Wan, Y. Meng, F. Zhang, D. Gu, Z. Chen, B. Tu, and D. Zhao., *J. Am. Chem. Soc*., 2006, **128**, 11652.

2 T. Kemmitt, N. I. Al-Salim, G. J. Gainsford, A. Bubendorfer, M. Waterland, *Inorg. Chem*., 2004, **43**, 6300.

3 R. Liu, Y. Ren, Y. Shi, F. Zhang, L. Zhang, B. Tu, and D. Zhao, *Chem. Mater*., 2008, **20**, 1140.

4 T. Yu, Y. Deng, L. Wang, R. Liu, L. Zhang, B. Tu and D. Zhao, *Adv, Mater.*, 2007, **19**, 2301.