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Supporting Information

A Mechanistic Study of Mesoporous TiO_2 Nanoparticle Negative Electrode Material with Varying Crystallinity for Lithium Ion Batteries

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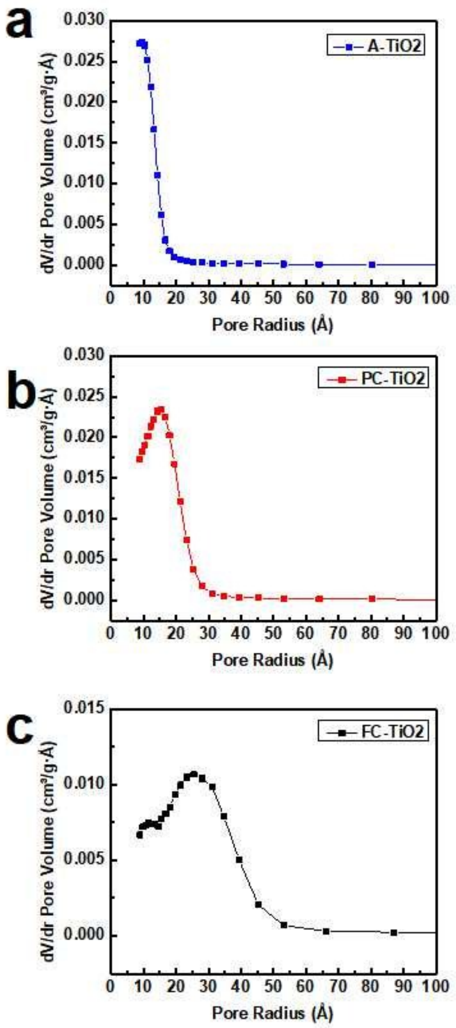

Fig. S1 Pore size distribution of TiO_2 nanoparticle samples.

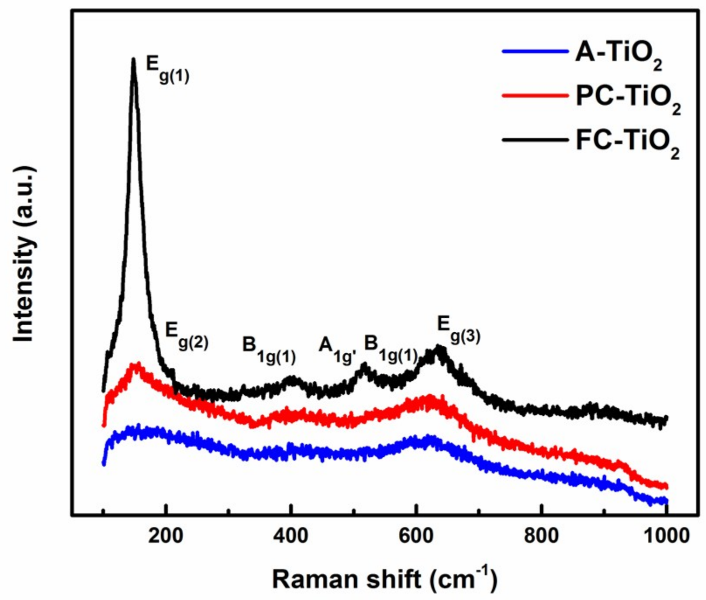

Fig. S2 Raman spectra of pristine mesoporous TiO_2 nanoparticle samples.

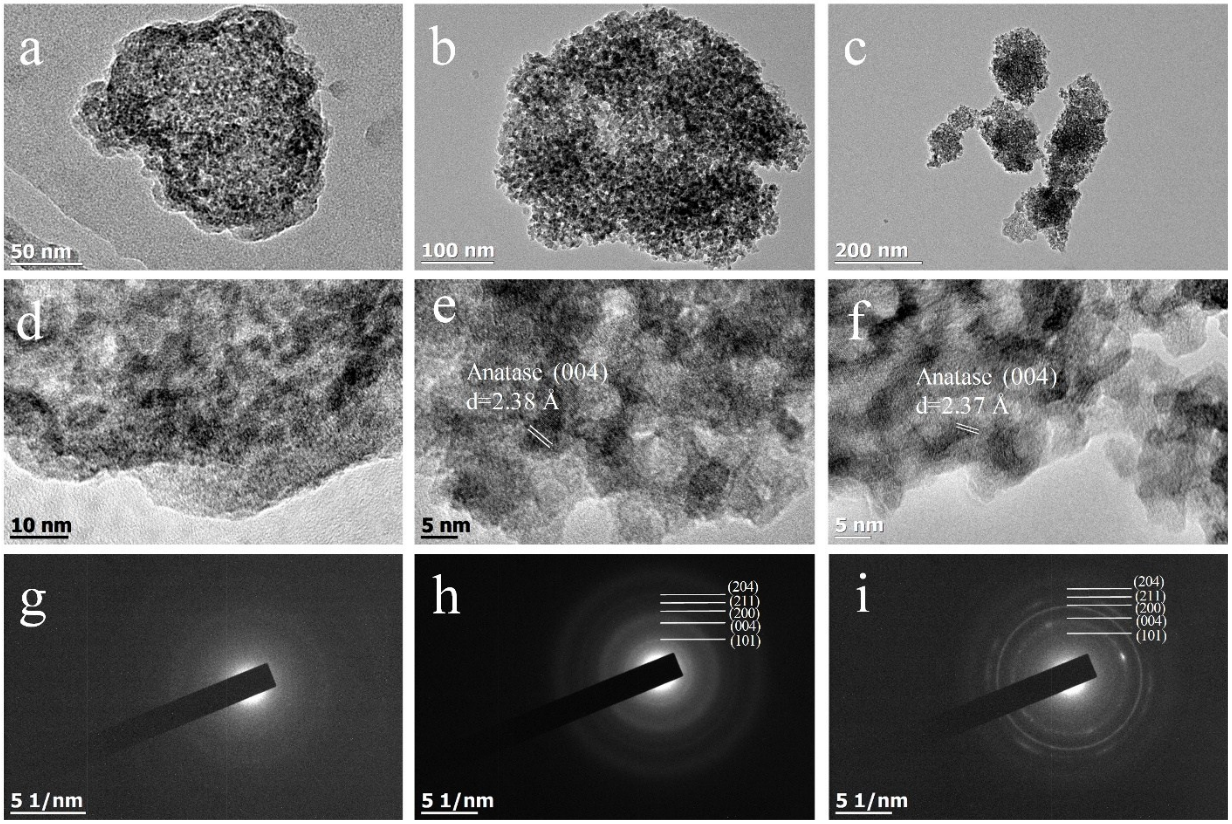

Fig. S3 TEM images of cycled electrodes: (a) A-TiO_2, (b) PC- TiO_2 and (c) FC- TiO_2. HRTEM images of (d) A-TiO_2, (e) PC- TiO_2 and (f) FC- TiO_2. And SAED patterns of (g) A- TiO_2, (h) PC- TiO_2 and (i) FC- TiO_2.

The diffusion coefficient can be expressed as the following equation: [1]

$$D_{Li+} = \frac{\pi}{4}\left(\frac{m_B V_M}{M_B S}\right)^2 \left(\frac{\Delta E_S}{\tau\left({dE_t}/{d\sqrt{\tau}}\right)}\right)^2, \tau \ll \frac{L^2}{D_{Li+}} \tag{1}$$

where m_B, V_M, M_B, S and τ are mass, molecular volume, molecular weight, active surface area and current pulse time of the electrode. If E versus $\sqrt{\tau}$ shows a linear behavior during the current pulse (Figure S2), the equation can be transformed into:

$$D_{Li+} = \frac{\pi}{4\tau}\left(\frac{m_B V_M}{M_B S}\right)^2 \left(\frac{\Delta E_S}{\Delta E_t}\right)^2, \tau \ll \frac{L^2}{D_{Li+}} \tag{2}$$

Where ΔE_S and ΔE_t for each titration are illustrated in Figure S2.

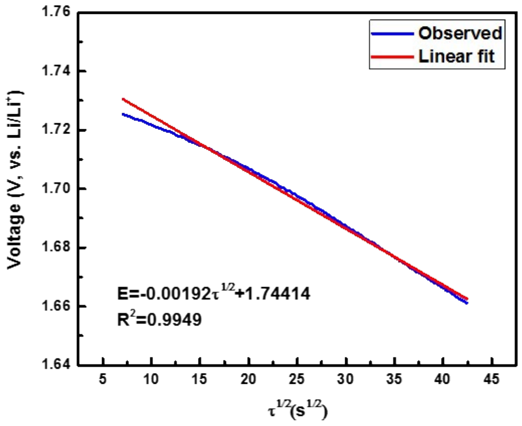

Fig. S4 Linear behavior of the E vs $\tau^{1/2}$ relationship.

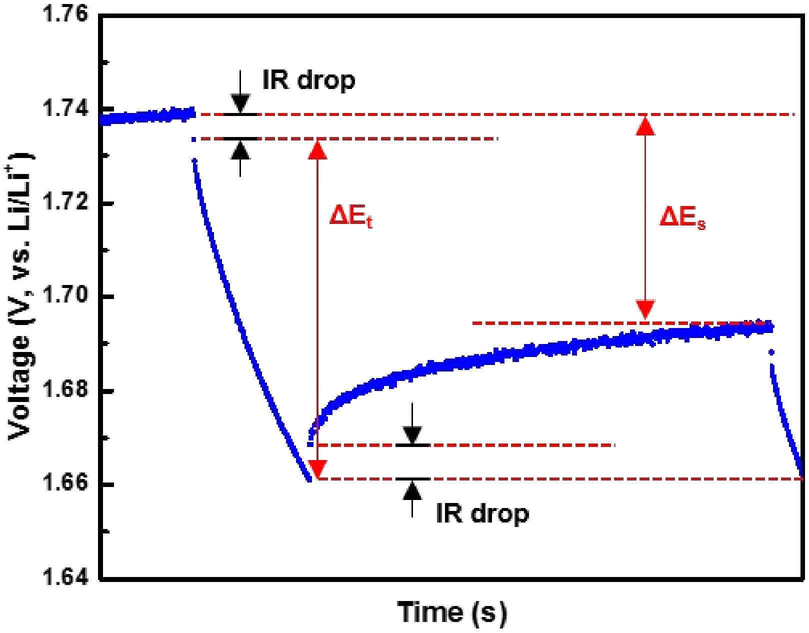

Fig. S5 Schematic of GITT technique.

References

1 Weppner, W., and Robert A. Huggins. *J. Electrochem. Soc.* 1977, **124**, 1569-1578.