Supporting Information

Superior shuttling of lithium and sodium ions in manganese-doped titania @ functionalized multiwall carbon nanotubes anode

Ata-ur-Rehman^{1,2,‡}, Ghulam Ali^{3,‡}, Amin Badshah¹, Kyung Yoon Chung³, Kyung-Wan Nam⁴, Muhammad Jawad⁵, Muhammad Arshad⁶, Syed Mustansar Abbas^{4*}

¹Department of Chemistry, Quaid-e-Azam University, Islamabad, Pakistan

² Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

³ Center for Energy Convergence, Korea Institute of Science and Technology, Seoul 136-791, Republic of Korea

⁴ Department of Energy and Materials Engineering, Dongguk University, 30, Pildong-ro 1gil, Jung-gu, Seoul 100-715, Republic of Korea

⁵ Health Physics Division, PINSTECH, P.O. Nilore, Islamabad, Pakistan

⁶ Nanoscience and Technology Department, National Centre for Physics, Islamabad, Pakistan

‡ These authors contributed equally

* Corresponding author. Tel.: +82-10-3192-4868; E-mail address: qau_abbas@yahoo.com (Syed Mustansar Abbas)



Figure S1 Charge/discharge voltage profile of (a) TiO₂ (b) TiO₂/MWCNTs (c) 3%Mn-TiO₂/MWCNTs (d) 7%Mn-TiO₂/MWCNTs for selected cycles measured at 0.1 C rate with a potential window of 1.0 to 3.0 V *vs* Li/Li⁺

The charge/discharge profile of bare TiO_2 , $TiO_2/MWCNTs$, 3% and 7% Mn- $TiO_2/MWCNTs$ electrode at selected charge-discharge cycles between 1.0 to 3.0 V at a current rate of 0.1 C demonstrate relatively higher capacities for Mn-doped and MWCNTs supported electrodes in comparison to bare TiO_2 .



Figure S2 Diffuse reflectance spectroscopy (DRS) band gap measurements of undoped and doped samples embedded on MWCNTs

The band gap energies (E_g) of samples are calculated by using UV-vis diffuse reflectance spectrometer (DRS) from 200-1200 nm wavelength. By applying Kubelka–Munk function ($\alpha = F(R) = (1-R)^2/2R$) diffuse reflectance is converted to absorbance coefficient, where F(R)' is Kubelka–Munk function , R' is reflectance and α ' is absorbance coefficient and then band gap energies are determined by using Tauc relationship (F(R) hv= A(hv-Eg)²) with hv' as photon energy. The band gap energy of TiO₂ slowly decreases with increases in Mn-doping along with MWCNTs interaction. The lowest band gap is observed for 5%Mn-TiO₂/MWCNTs with a maximum density of conduction electrons contributing towards the higher specific capacities of this electrode system.



Figure S3 Cycling performance (charge capacities) per volume *vs* cycle number and coulombic efficiency of samples (a) within a potential window of 1.0 to 3.0 V *vs* Li/Li⁺, and (b) within a potential window of 0.01 to 3.0 V *vs* Na/Na⁺