Supplementary information

Investigation of Synergistic Effect of Defects Rich V_2O_5/MWCNTs Heterostructure for improved electrochemical Performance of Supercapacitor

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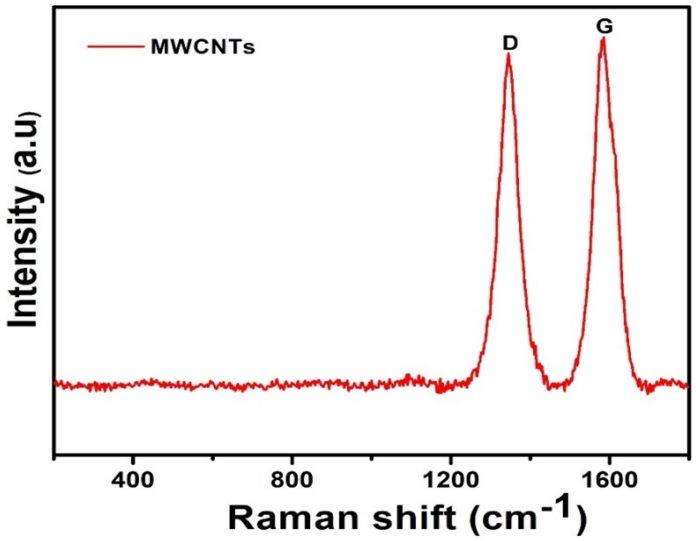

Fig. S1. Raman spectra of MWCNTs

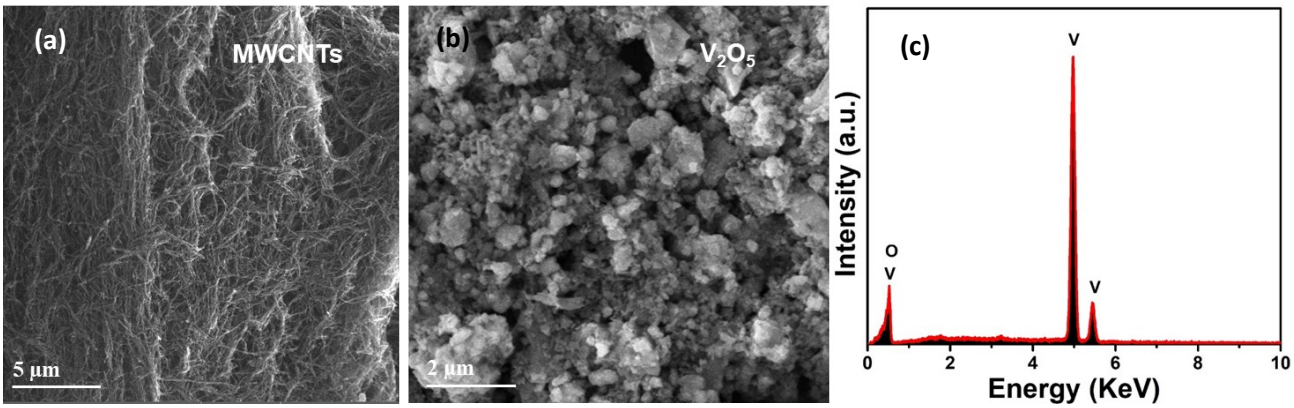

Fig. S2. SEM image of (a) MWCNTs (b) V_2O_5 and (c) Corresponding EDX spectrum of V_2O_5.

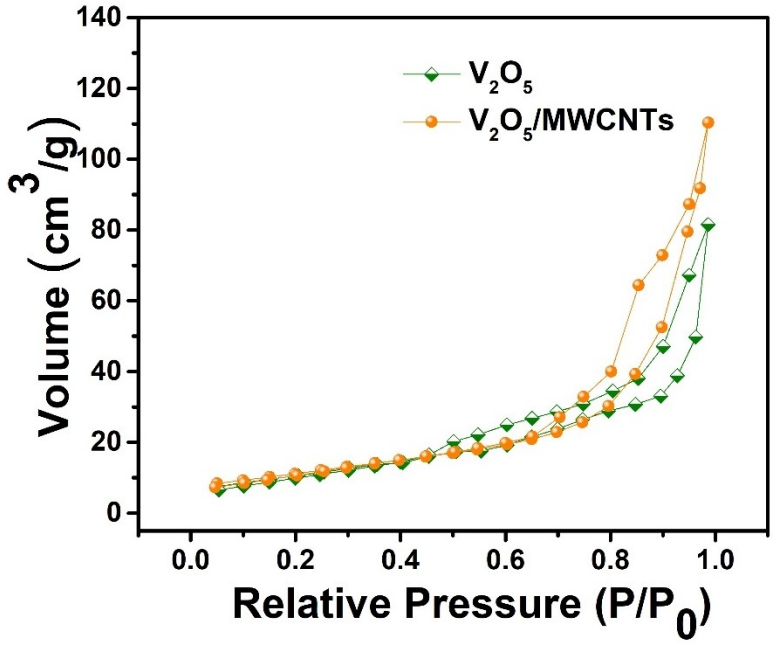

Fig. S3. BET surface area of V_2O_5 and V_2O_5/MWCNTs heterostructures.

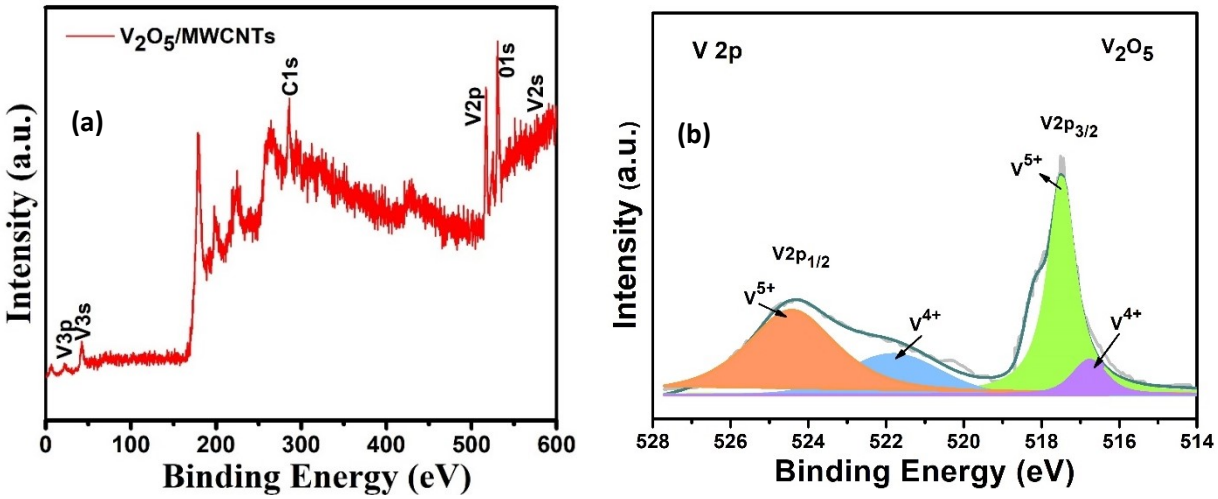

Fig. S4. (a) XPS survey spectrum of V_2O_5/ MWCNTs heterostructure (b) High resolution spectrum of V 2p peak of V_2O_5 nanostructure.

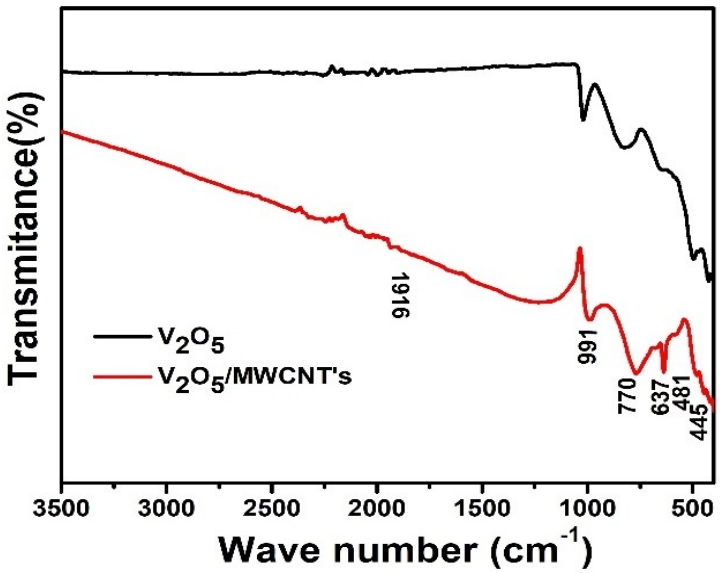

Fig. S5. FTIR spectra of V_2O_5 and V_2O_5/MWCNTs nanostructures.

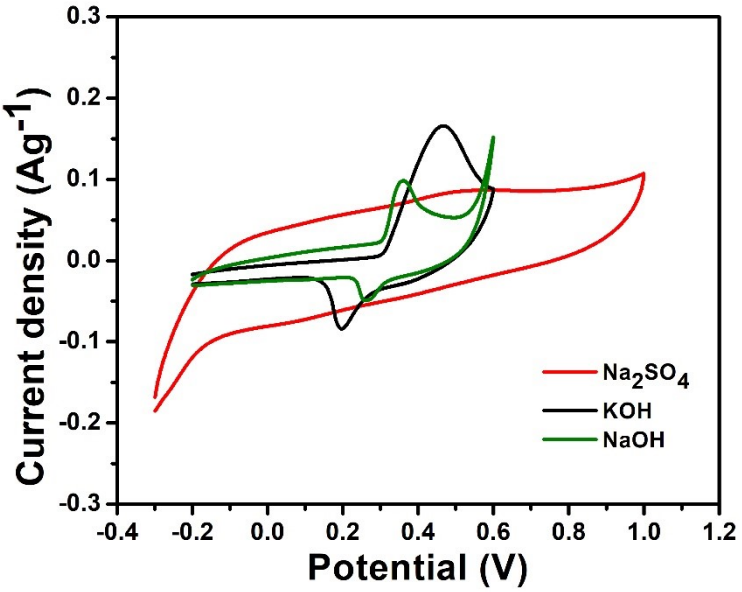

Fig. S6. CV response of V_2O_5/MWCNTs electrode in different 1 M electrolytes.

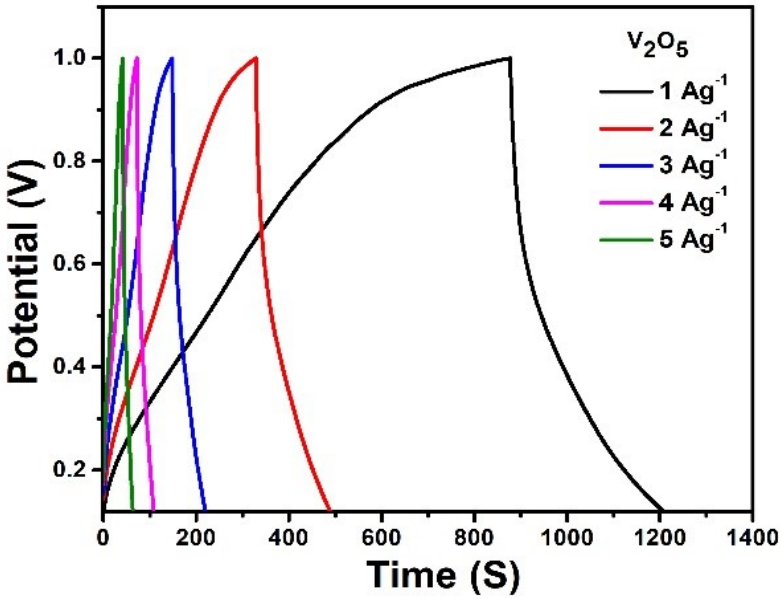

Fig. S7. GCD curves of V_2O_5 electrode at different current densities.

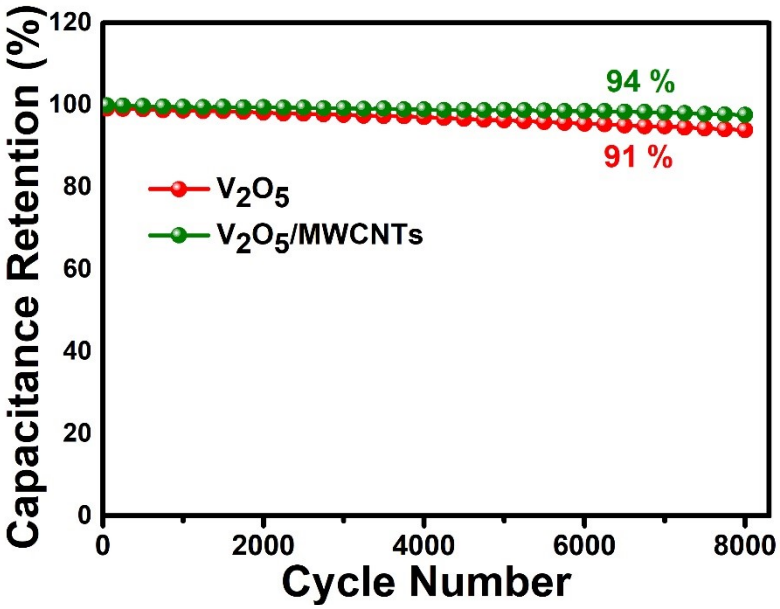

Fig. S8. cyclic stability of V_2O_5 and V_2O_5/MWCNTs electrodes at 2 Ag^{-1}.

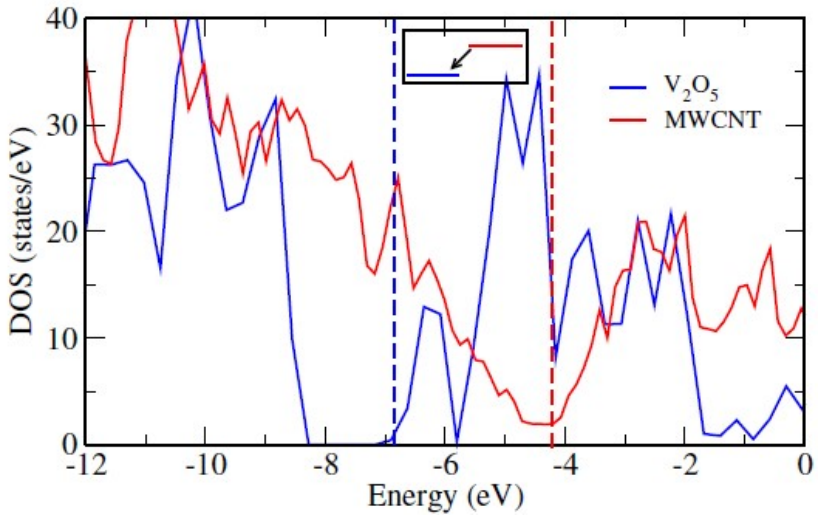

Fig S9: Total density of states of V_2O_5 and MWCNT, calculated with reference to the vacuum level of each material. The dashed vertical lines represent the conduction band minima for V2O5 (blue) and Fermi level for MWCNT (red). The inset schematically highlights the favorable charge transfer from the MWCNT to V_2O_5.

DFT Explanation

Fig. S8 depicts total density of states (TDOS) for (4,4)@ (8,8)@ (12,12) MWCNT and experimentally observed (110) surface of V_2O_5, calculated with GGA. Note that TDOS is referenced to the vacuum level of each material to provide a clear understanding of energy level alignment at the interface. As evident, the Fermi level (E_F) of MWCNT is significantly higher in energy than the conduction band minima of V_2O_5. Such energy level alignment will facilitate electron transfer from MWCNT to V_2O_5 as discussed in the main text (see also inset of Fig.S8). Furthermore, V_2O_5 has a large bandgap (from -8.2 eV to -6.9 eV, Fig. S8) whereas bandgap is closed for MWCNT. These results clearly indicate that MWCNT/ V_2O_5 heterostructure will have higher conductivity as compared to pristine V_2O_5, as discussed in the main text.

Table. S1. Comparative analysis of fitted parameters of V_2O_5/MWCNTs and V_2O_5 electrodes.

Material	**R_s (Ω)**	**R_{ct} (Ω)**
V_2O_5/MWCNTs	1.4	62. 3
V_2O_5	2.9	144.4