Supporting Information

Supercapacitive behaviour of a novel nanocomposite of 3,4,9,10-perylenetetracarboxylic acid incorporated Captopril-Ag Nanocluster decorated on graphene nanosheets

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Contents

Preparation of Nb_2O_5 nanostructure

A homogenous white paste of Nb_2O_5 (0.5 g) was prepared in 2 mL of oleylamine. The white paste was dispersed in dil. HNO_3 (1 mL of conc. HNO_3 dissolved in 10 mL of distilled water). It was stirred for another 20 min. The whole dispersion was transferred into a 100 mL teflon autoclave. The autoclave was kept in a muffle furnace at a constant temperature of 180 °C for 20 h. After cooling the autoclave to room temperature, the resultant mixture was centrifuged at 14500 rpm. The supernatant liquid was discarded and the solid product was washed multiple times with hexane. The solid product was dried at 80 °C.

Synthesis of PTCDA/Nb_2O_5

0.195 g of Nb_2O_5 nanostructure was mixed with 0.0354 g of PTCDA/PVP microstructure in 50 mL of DMSO. The suspension of the mixture in DMSO was ultrasonicated using a pulsed ultrasonicator for 1 h. Then the suspension was kept under constant stirring for 24 h. The product was precipitated by adding excess acetone and separated by centrifugation at 14500 rpm. The solid product was washed multiple times with ethanol and water. Solid purple colored product was dried in vacuum oven at 80°C.

Characterization of Nb_2O_5 and PTCDA/Nb_2O_5

SEM analysis: The morphology and structures of Nb_2O_5 and PTCDA/Nb_2O_5 were characterized by SEM micrograph (Fig S2). Nanostructure of the dimension of ~200 nm can be seen in Fig. S2c.

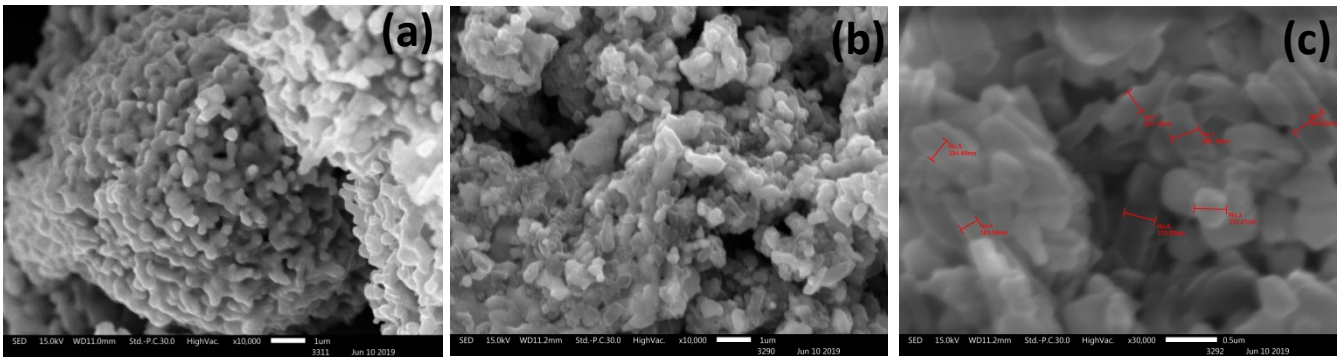

Figure S1. SEM images of (a) Nb_2O_5 nanostructure; (b) and (c) PTCDA/Nb_2O_5 at scale of 1 μm and 0.5 μm respectively

XRD spectra of Nb_2O_5 and PTCDA/Nb_2O_5

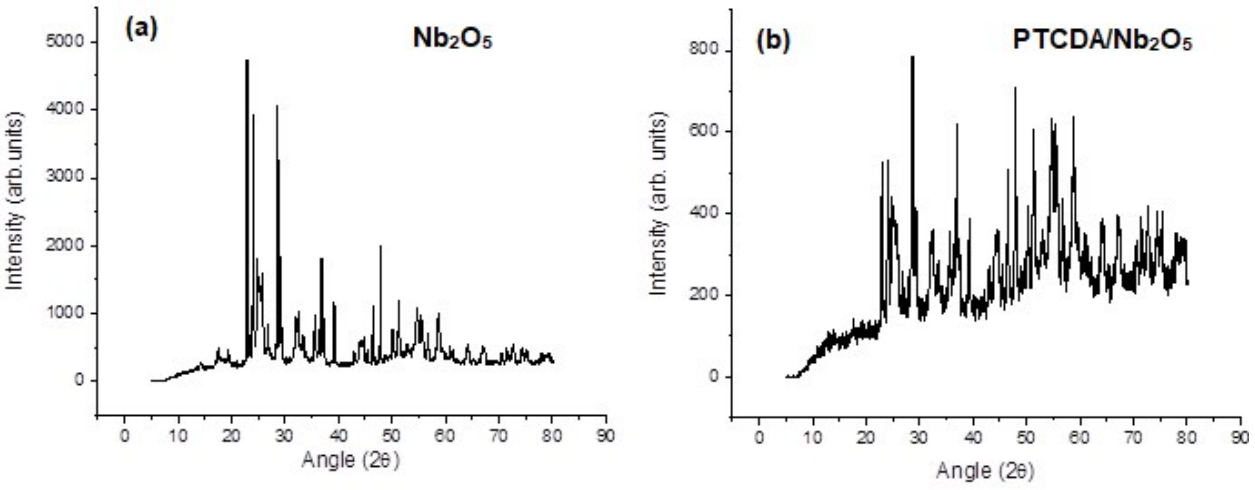

Figure S2. XRD spectra of (a) Nb_2O_5 and (b) PTCDA/Nb_2O_5

The nanocomposite PTCDA/Nb_2O_5 was further characterized by X-ray diffraction (Fig. S3). The diffractogram contains all the characteristic peaks of orthorhombic (T-phase) (JCPDS No. 00-027-1313) and monoclinic (H-phase) (JCPDS No. 00-027-1312) phase of Nb_2O_5. The peaks of PTCDA can be found at 24.7°, 27.5° and 32°. The presence of all the characteristic phases of PTCDA and Nb_2O_5 suggests the successful preparation of the nanocomposite.

FTIR spectra of Nb_2O_5 and PTCDA/Nb_2O_5

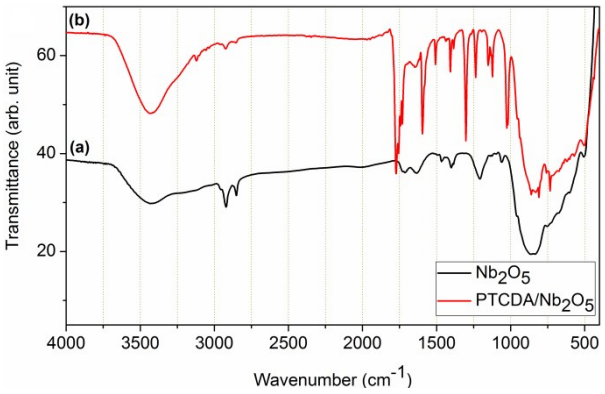

Figure S3. FTIR spectra of (a) Nb_2O_5 (b) PTCDA/Nb_2O_5

Synthesis of TiO_2/Nb_2O_5/AgNC

The nanocomposite TiO_2/Nb_2O_5/AgNC was prepared by following the procedure as described by elsewhere (T. Goswami et. al. ChemistrySelect, DOI: 10.1002/slct.201901097). In brief, 130 mg captopril was dissolved in a mixture of 15 mL of methanol and 15 mL of ethanol. Then, 59 mg of silver trifluoroacetate was added into it. It was kept under stirring at 400 rpm for 30 min. The pH of the solution was then raised to 9 by adding 0.2 N CsOH. Into this suspension, 160 mg of $TiO2/Nb_2O_5$ nanocomposite as prepared previously was added. After 20 min of stirring, 200 mg of tetramethylammonium borohydride (TMAB) was added at once. It was stirred for 2h and then 500 μL of H_2O_2 was added. The mixture was allowed to stir for 1 h. The whole solution was poured into excess (30 mL) acetone to precipitate the product. It was then centrifuged at 14500 rpm, the supernatant was discarded and the solid product was repeatedly washed with water and ethanol. The product was then dried in an oven at 60°C.

The as-prepared nanocomposite was characterized by HRTEM measurement. As can be seen in the TEM micrograph (Fig. S5) ~ 2-3 nm silver nanoclusters, ~ 8-10 nm TiO_2 nanoparticles are anchored in the surface of Nb_2O_5. The electrochemical capacitance property of this nanocomposite was measured in the present study.

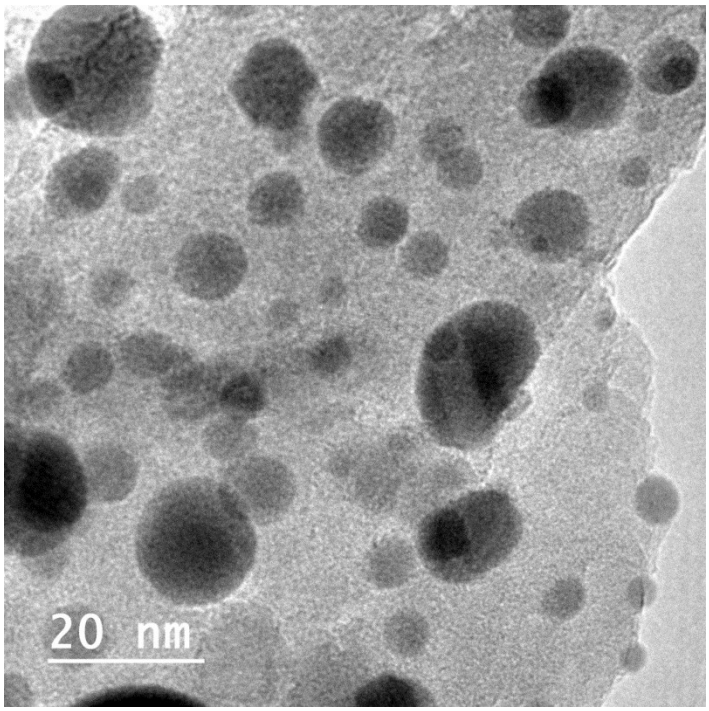

Figure S4: HRTEM micrograph of TiO_2/Nb_2O_5/capt-AgNC

Fig. S5 shows the XRD pattern of as-prepared exfoliated graphene nanosheets. The peaks at 25.9° and 43.6° correspond to (002) and (100) lattice planes, confirming the formation of reduced graphene oxide.

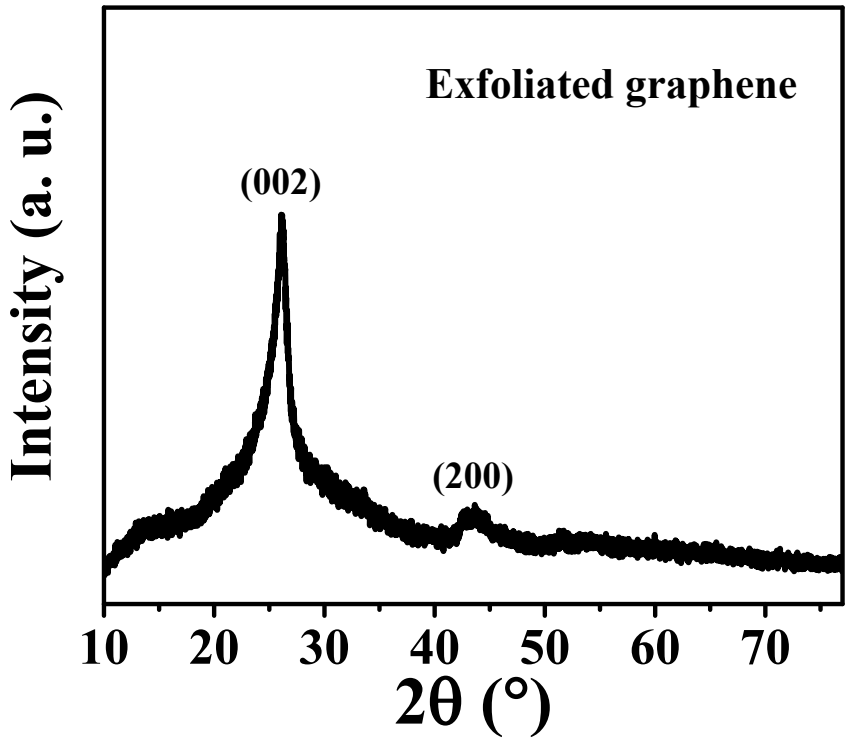

Figure S5. X-Ray Diffraction pattern of as prepared exfoliated graphene nanosheets

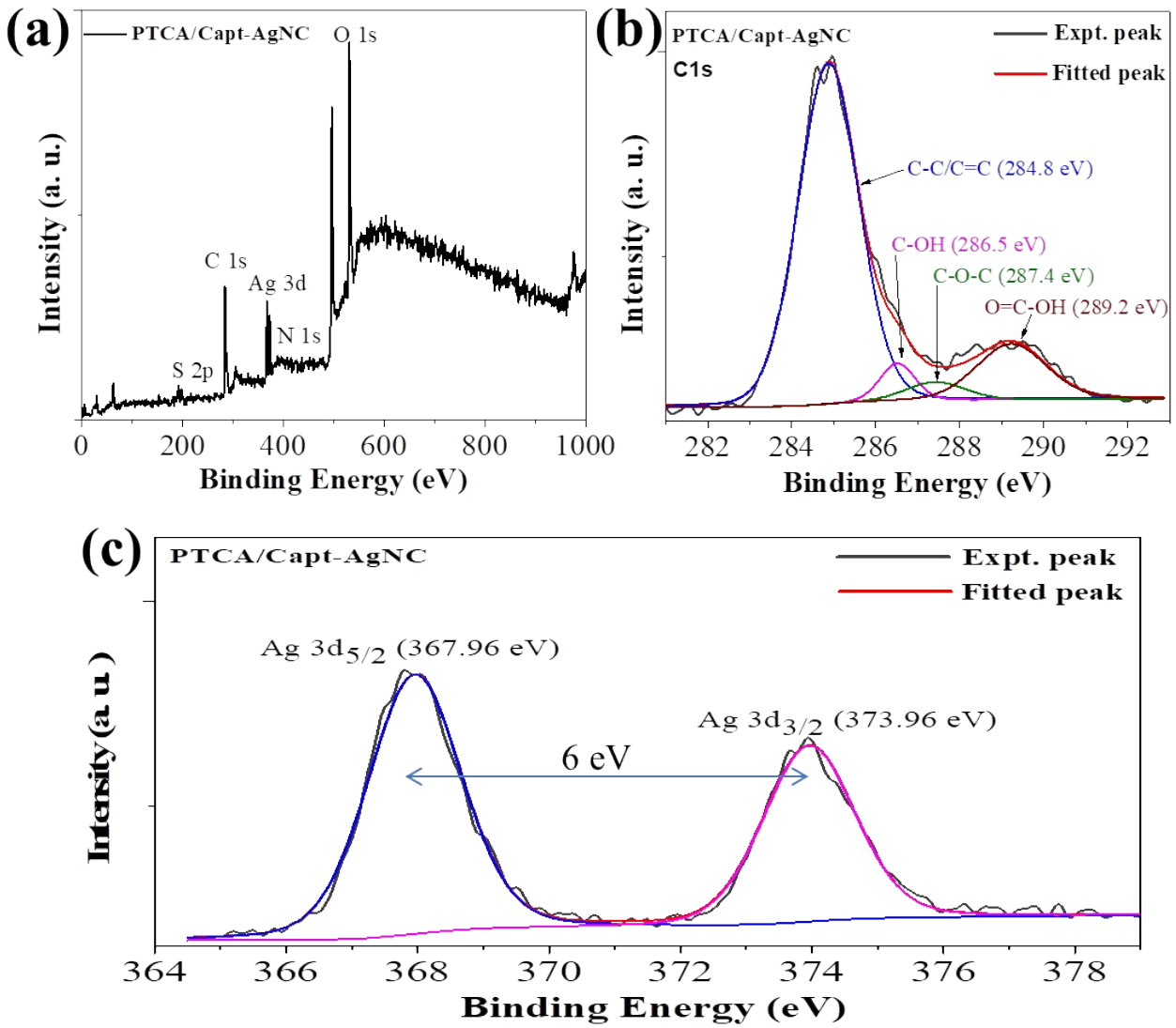

Figure S6. (a) Survey XPS spectra and deconvolution of XPS peak of (b) C 1s and (c) Ag 3d of PTCA/capt-AgNC.

Table S1: The detailed values of randles equivalent circuit elements.

Sr. No.	Element	Value
1.	R_s	5.809
2.	CPE1-T	2.2814E-5
3.	CPE1-P	0.72199
4.	R_{ct}	344.8
5.	Wo1-R	9298
6.	Wo1-T	0.00029501
7.	Wo1-P	2.785