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Molybdenum Disulfide (MoS_2) along with Graphene Nanoplatelets (GNPs) Utilized to Enhance the Capacitance of Conducting Polymers (PANI and PPy)

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Material Characterization of $Mo(dtc)_4$

Synthesized *Tetrakis*(diethyldithiocarbamato) molybdenum (IV) *i.e.* $Mo(dtc)_4$ was characterized by elemental analysis, FT-IR and thermogravimetric analyses as discussed below.

Elemental Analysis

The theoretical values calculated (*i.e.* Anal. Calc.) for $Mo(dtc)_4$; $C_{20}H_{40}N_4S_8Mo$ are C, 34.9; H 5.9; N, 8.1% [1, 2] and in our synthesized $Mo(dtc)_4$ the values found are C, 34.9; H, 5.9; N, 8.1% using an organic elemental analyzer of Thermo Scientific Flash 2000.

Fourier Transform Infrared Spectroscopy (FT-IR)

FT-IR spectrum of $Mo(dtc)_4$ (Figure S1) is showing the peaks/bands at 2971, 2933, 2869, 1516, 1491, 1455, 1428, 1376, 1352, 1269, 1210, 1145, 1095, 1074, 1003 and 990 cm^{-1} which are consistent with earlier reports [1-3]. Three basic regions exist in infrared spectra of dithiocarbamato complexes;

- The first main region extents from 1450 to 1550 cm^{-1} and account for thioureide (NCSS) band which typically occurs betwixt C-N and C=N band. The absorption band at 1500 cm^{-1} is attributed as arising from polar structure —NCS_2.
- The second region (1070-930 cm^{-1}) is descriptive of mode of coordination in dithiocarbamato moiety (CSS).
- The third region around 350-400 cm^{-1} is attributed to M-S bonds. [1-3]

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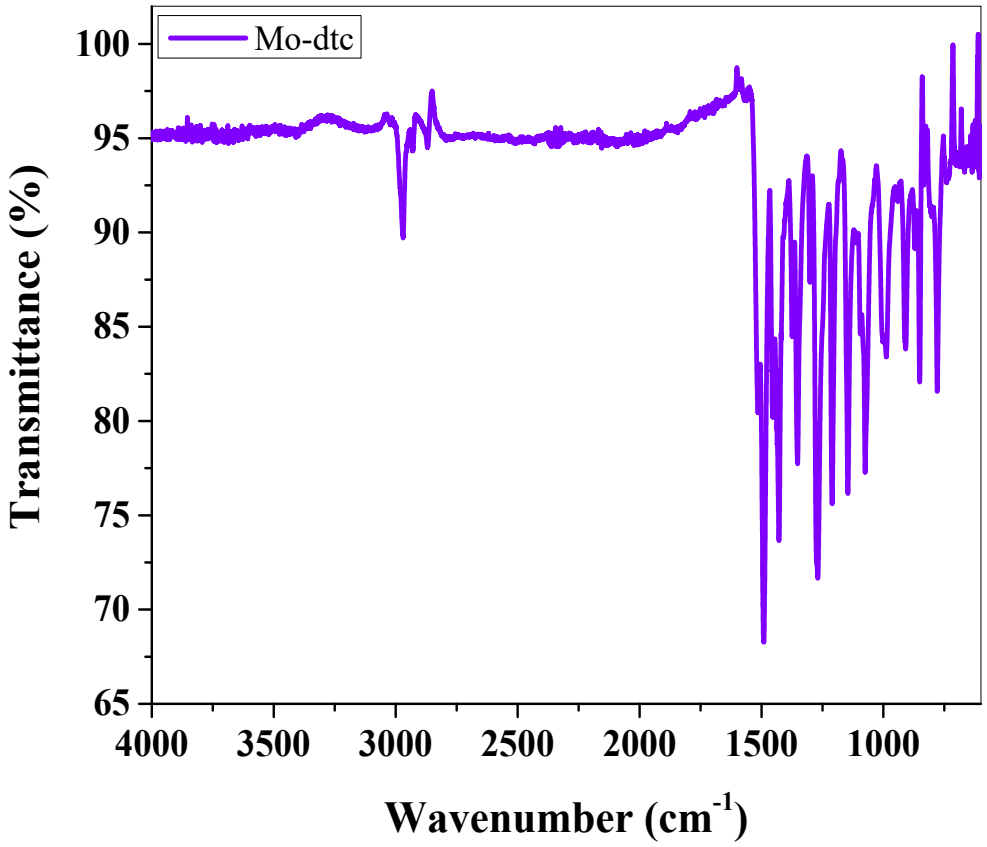

Figure S1: Fourier transform infrared (FT-IR) spectroscopy of $Mo(dtc)_4$.

Thermogravimetric Analysis (TGA)

Figure S2 displays the TGA of $Mo(dtc)_4$ under the environment of nitrogen. Three stages of decomposition take place at 151, 233, and 352 °C. The first -7.2 % decomposition step at 151 °C is due to the loss of ethylene (-4.0% calculated weight% loss) while -41.8% second step at 233 °C is due to two diethyldithiocarbamate molecules (-42.9% calculated weight% loss). The remaining material is a black solid with a residual weight percent of 28.3% after the third decomposition process (-22.7%). This thermal decomposition of $Mo(dtc)_4$ consequences to produce (23.5% calculated weight%) pure MoS_2, while aditional 4.8% is due to decomposed ligand contamination. [4]

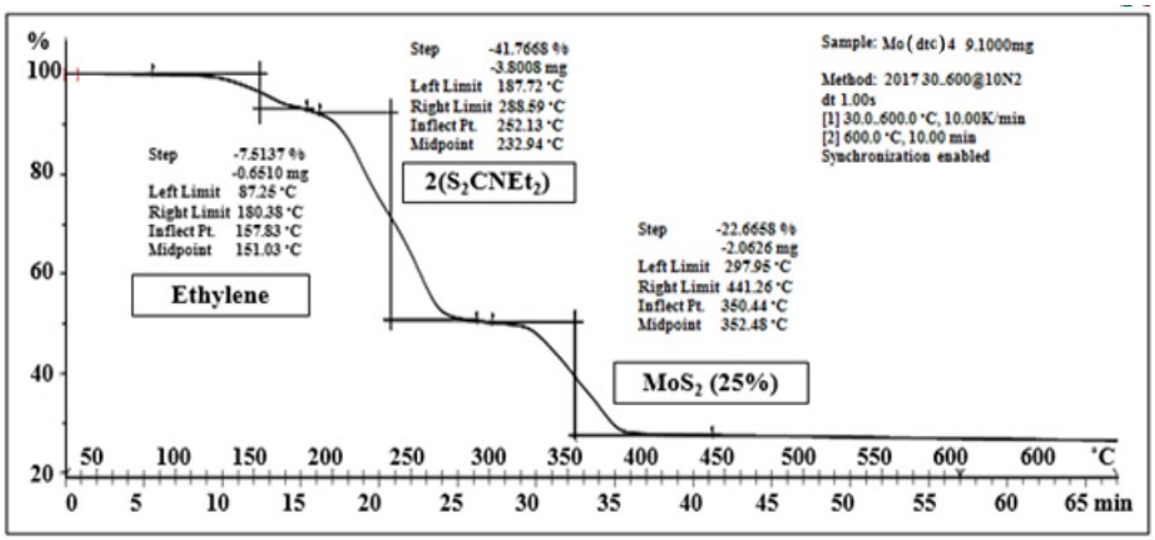

Figure S2: Thermogravimetric analysis (TGA) of $Mo(dtc)_4$.

Raman Analysis of MoS_2 melt

Raman spectra (Figure S3) indicates that thermolysis process under argon inert environment yields MoS_2 with A_{1g} out-of-plane mode centered at 361 cm^{-1} and E^1_{2g} in-plane mode seen at 334 cm^{-1} ($\Delta\nu$ = 27 cm^{-1}). [5] Phonon confinement may be the reason for softening of two modes and peaks broadening, which depicted that achieved resultant MoS_2 material is of few layers. [6, 7]

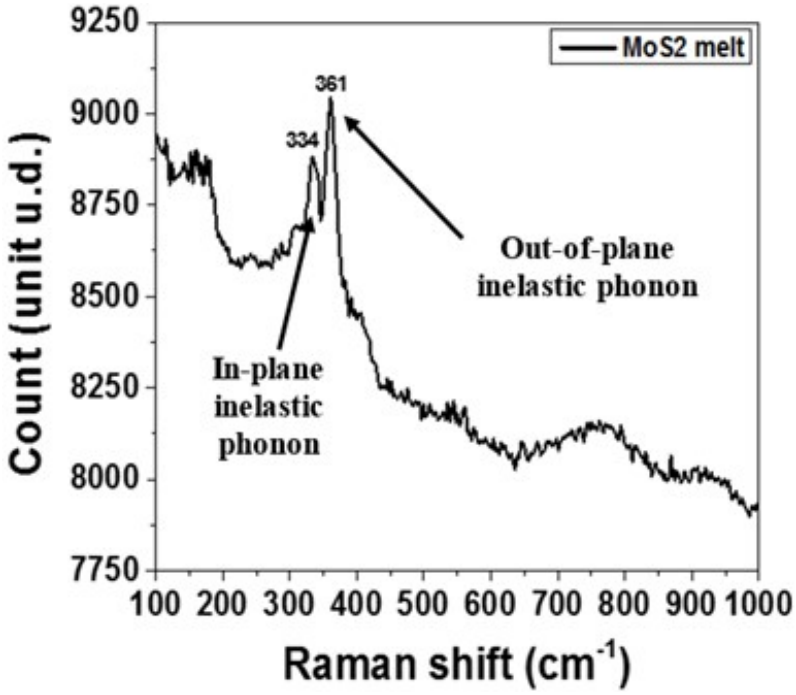

Figure S3: Raman analysis of MoS_2 melt.

Electrochemical Studies

Cyclic Voltammetry (CV)

CV at Various Scan Rates

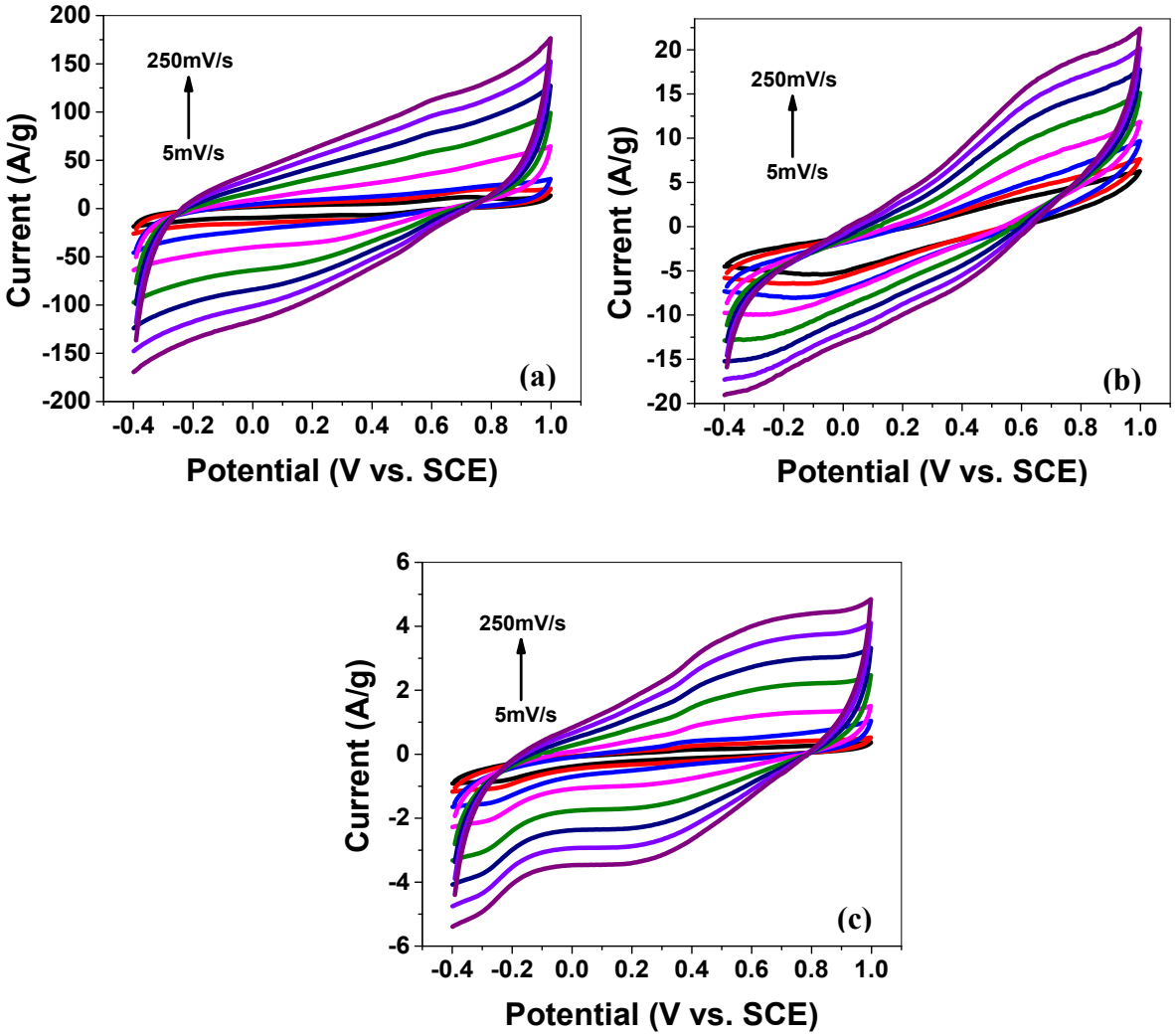

Figure S4: Cyclic voltammetry (CV) of (a) M5, (b) mPP and (c) mP at different scan rates on GCE in 1M H_2SO_4 vs. SCE.

Cyclic Stability for 50 Cycles of CV

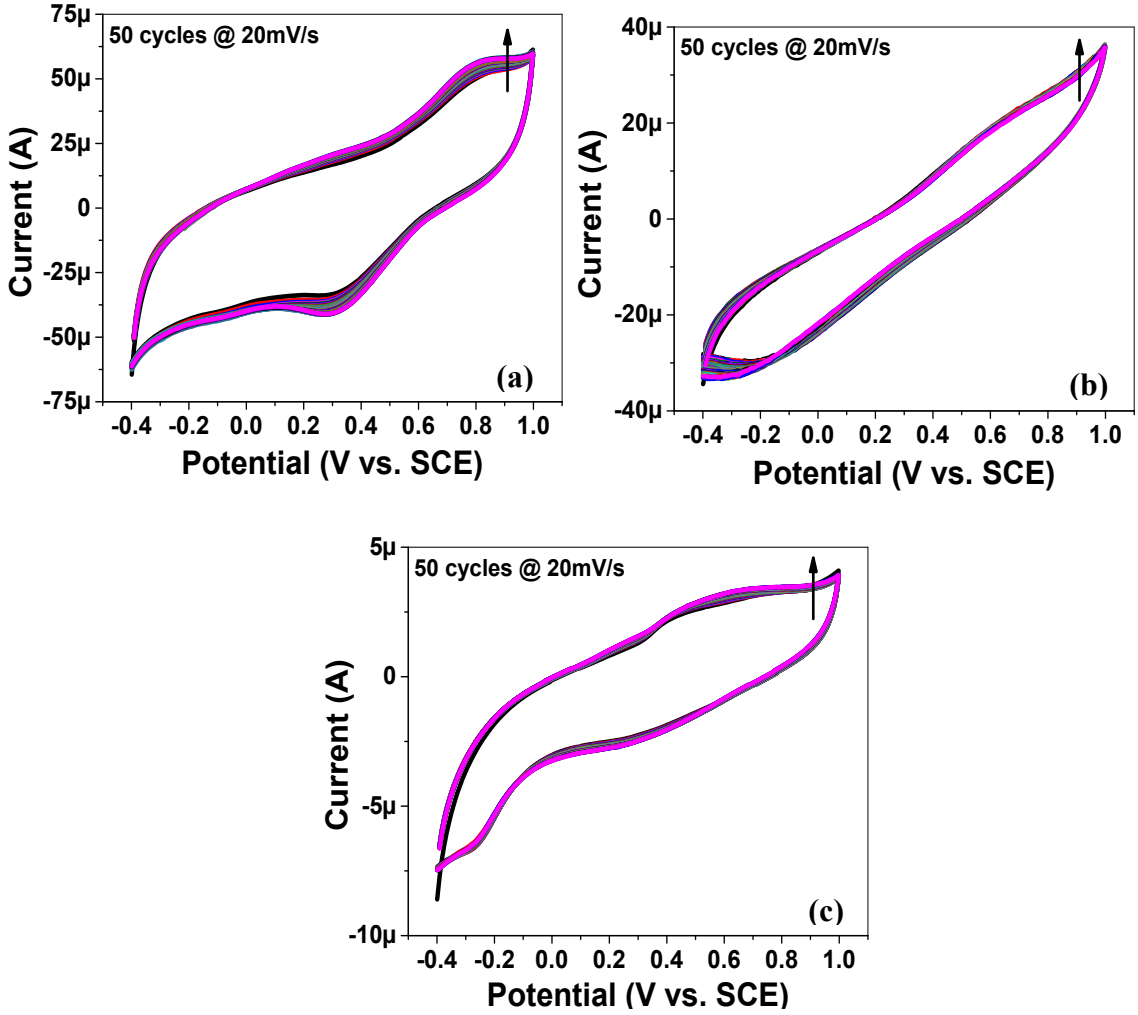

Figure S5: Cyclic voltammetry (CV): cyclic stability of (a) M5, (b) mPP and (c) mP at scan rate of 20mV/s for 50 cycles on GCE in 1M H_2SO_4 electrolyte vs. SCE.

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EIS (Electrochemical Impedance Spectroscopy)

EIS Nyquist plots

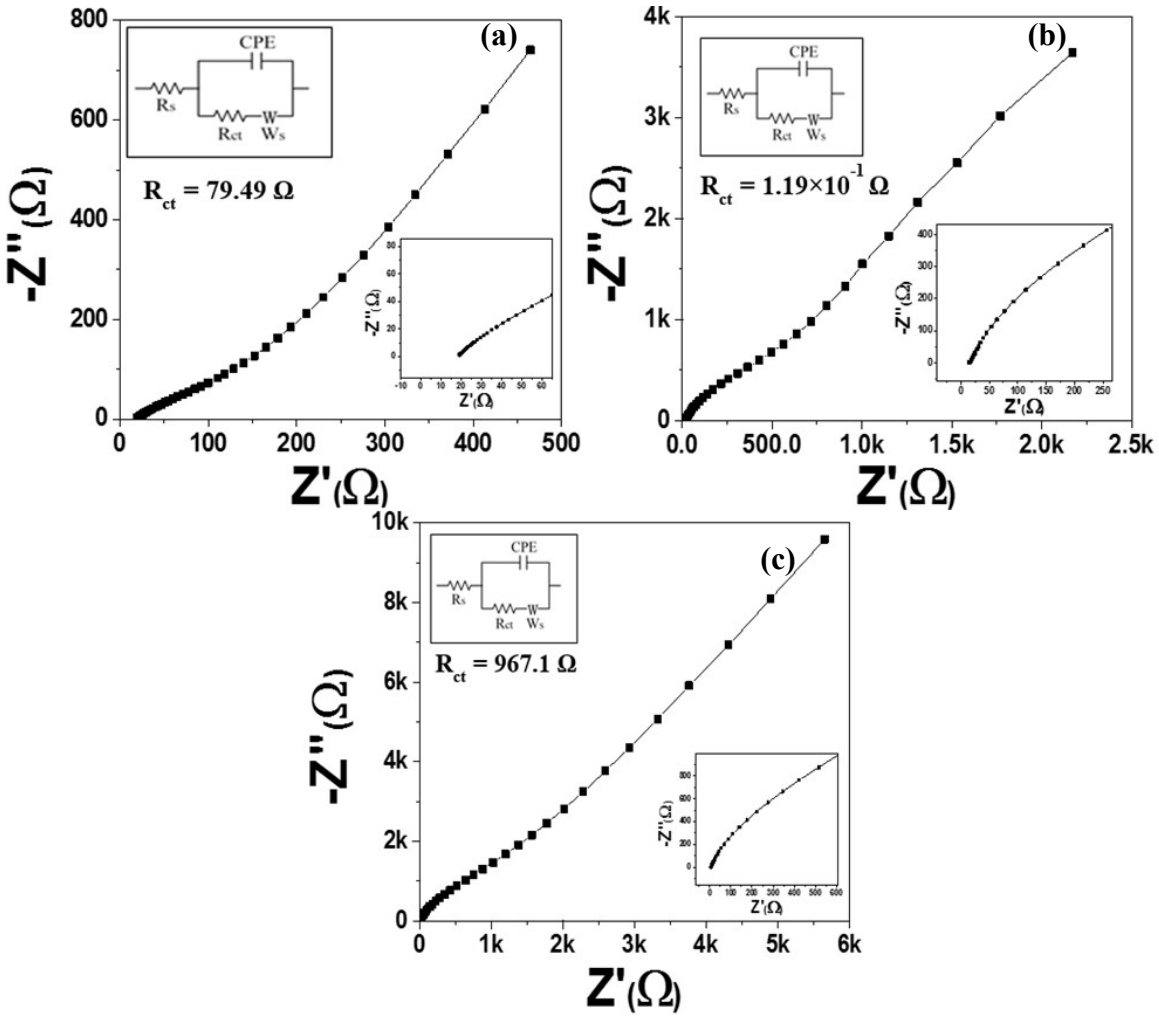

Figure S6: EIS Nyquist plots of (a) M5, (b) mPP and (c) mP vs. OC in 1M H_2SO_4 electrolyte with equivalent circuit diagram.

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EIS Bode plots

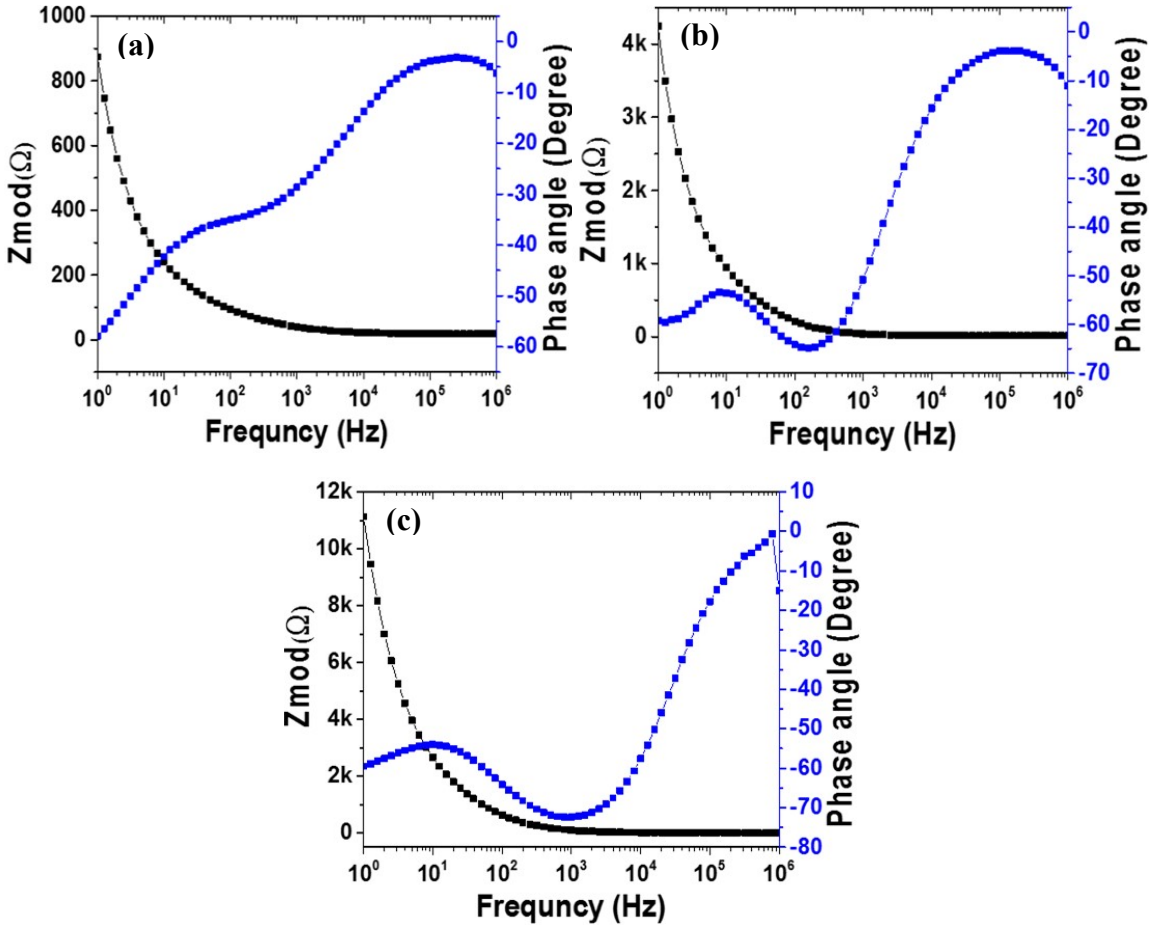

Figure S7: EIS (Electrochemical Impedance Spectroscopy): Bode plots of (a) M5, (b) mPP and (c) mP vs. OC (open circuit) at 10mv rms AC perturbation (in 1M H_2SO_4 electrolyte).

Galvanostatic Charge/Discharge (GCCD) Measurements

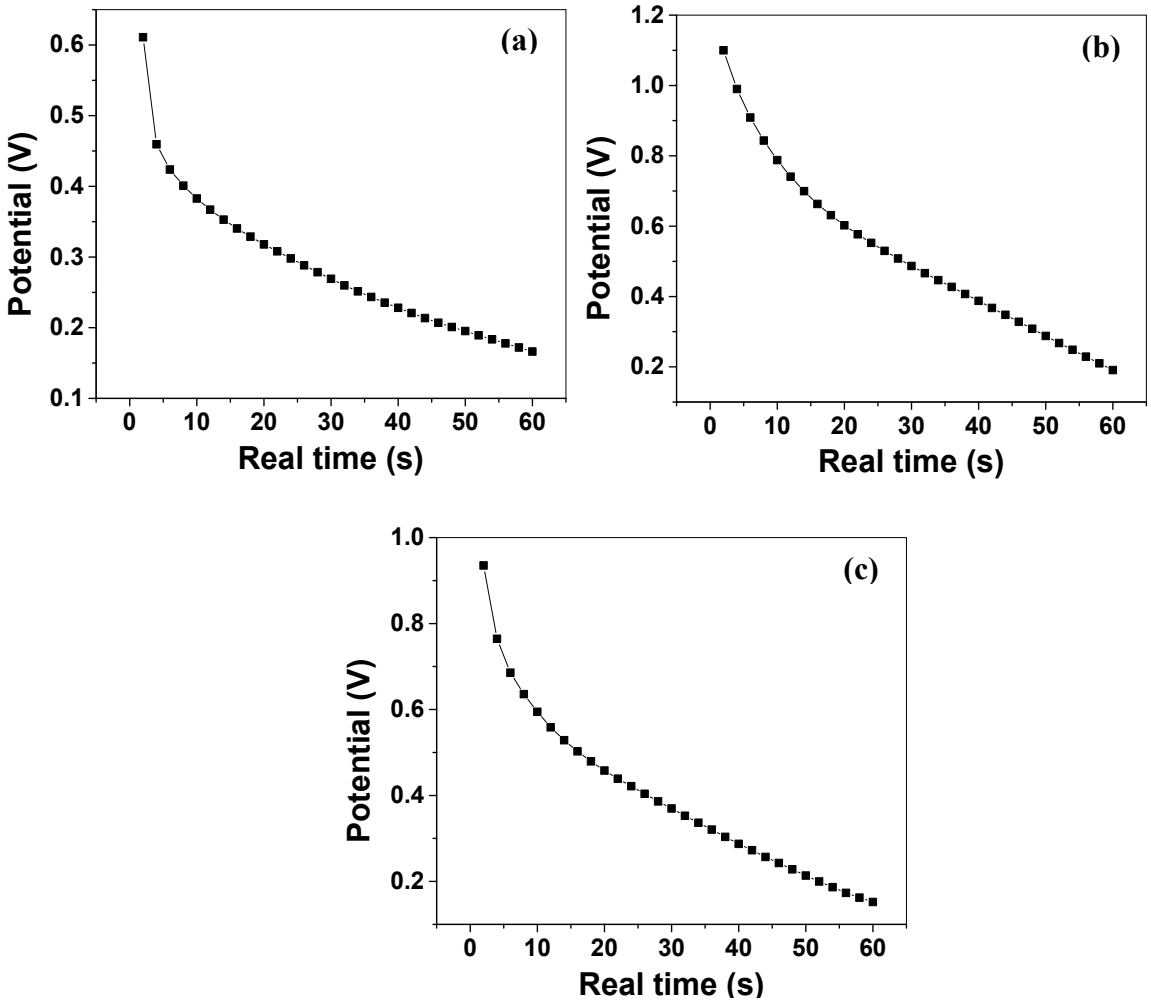

Figure S8: GCCD (Galvanostatic cyclic charge discharge): Discharge curve of (a) M5, (b) mPP and (c) mP Potential vs. real time (at charge density= 0.57 A/g) in 1M H_2SO_4 electrolyte.

Galvanostatic Charge/Discharge (GCCD) Measurements at different charge densities

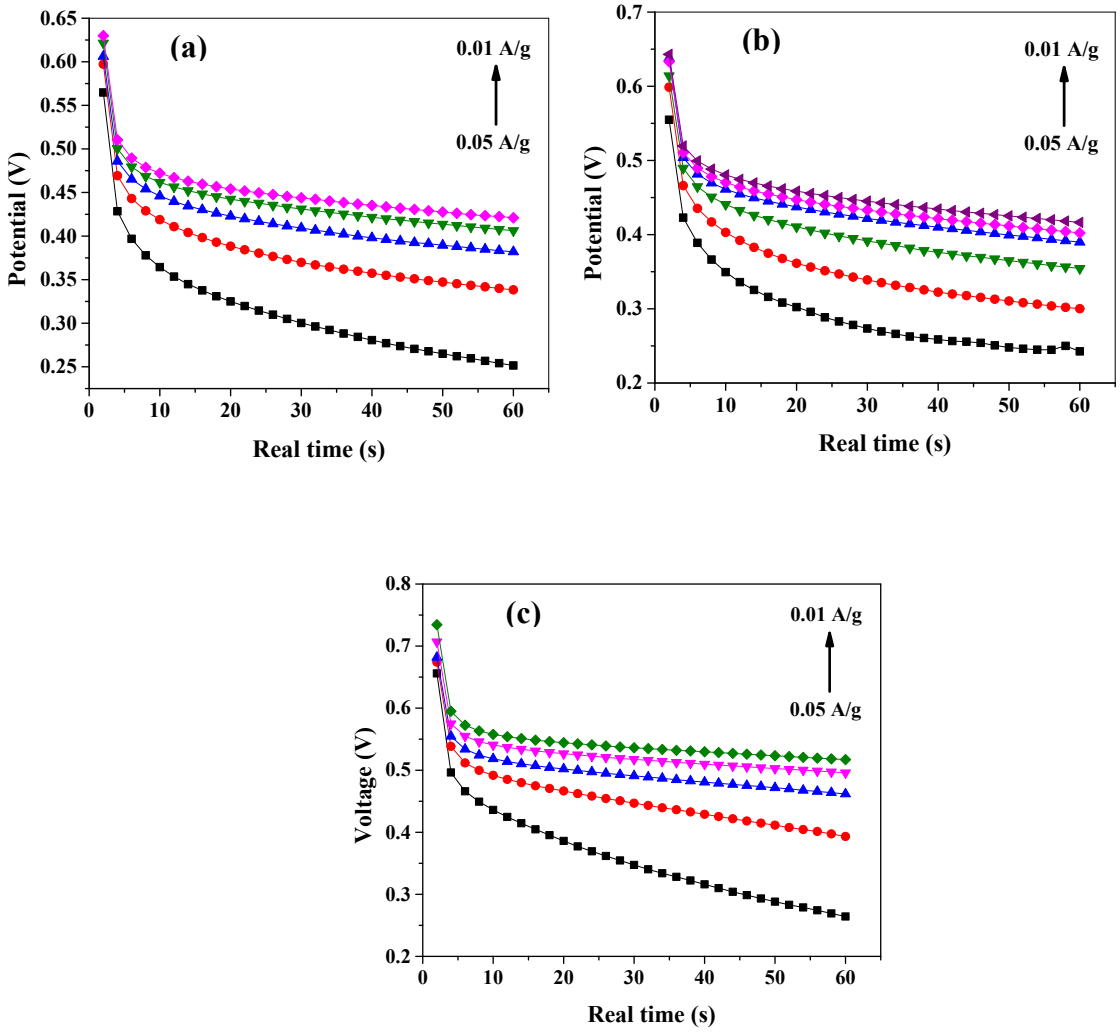

Figure S9: GCCD (Galvanostatic cyclic charge discharge): Discharge curve of (a) MoS_2 melt 5mPP, (b) MoS_2 melt 5mP and (c) MoS_2 melt Potential vs. real time at different charge densities in 1M H_2SO_4 electrolyte.

Galvanostatic Charge/Discharge (GCCD) Capacitance retention of MoS_2 melt 5mPP vs. cycle number for 10,000 cycles

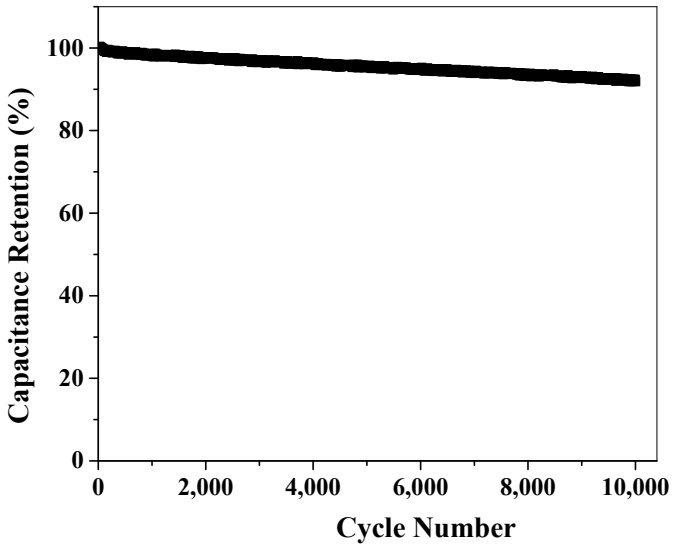

Figure S10: GCCD: Capacitance retention of MoS_2 melt 5mPP vs. cycle number for 10,000 cycles (in 1M H_2SO_4 electrolyte).

Capacitance retention of MoS_2 melt 5mPP for 10,000 charge-discharge cycles in 1M H_2SO_4 electrolyte is shown in Figure S10. The composite demonstrates improved charge storage performance and excellent cyclic stability (91.87% capacitance retention at 0.57 A/g after 10,000 cycles).

Raman Analysis of M5-Graphene nanoplatelets

Raman spectra for M5-Graphene nanoplatelets is shown in Figure S11.

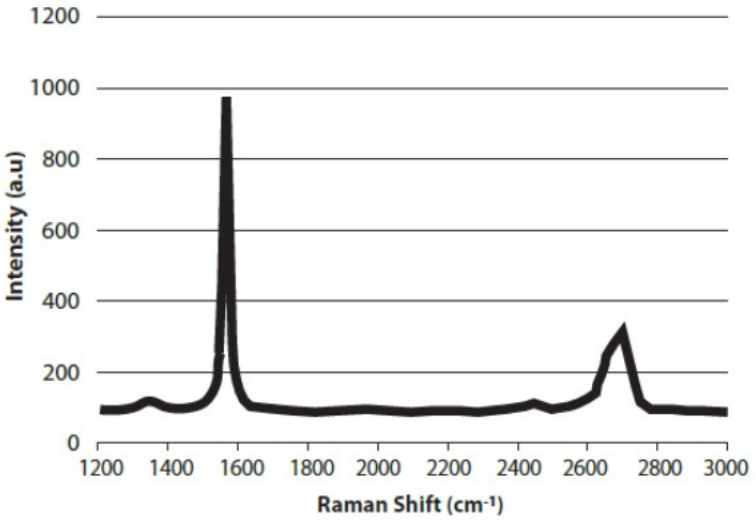

Figure S11: Raman analysis of M5.

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Notes and References

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