Supporting Information

Polypyrrole-promoted rGO-MoS_2 nanocomposite for enhanced photocatalytic conversion of CO_2 and H_2O to CO, CH_4 and H_2 products

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Experimental:

Synthesis of graphene oxide sheets using improved Hummer's method: In a typical experiment, 3 g of graphite powder was added to 400 mL of a concentrated acid mixture (H_3PO_4/H_2SO_4:1/9 v/v) and stirred for a 15 min. $KMnO_4$ (6 weight equivalent of graphite) was then added to the above mixture and stirred at 50°C for 14 h. After completion, the reaction was cooled naturally and then poured on ice ~500 mL with 5 mL of H_2O_2 (30 %). To avoid Mn impurities, the solution was further diluted with deionized (DI) water and centrifuged using water and diluted HCl to obtain dark a brown product as graphite oxide. This product was re-dispersed in D.I. H_2O and sonicated for 2 h to get graphene oxide nanosheets. In Fig. S1, XRD confirms the successful formation of graphene oxide.

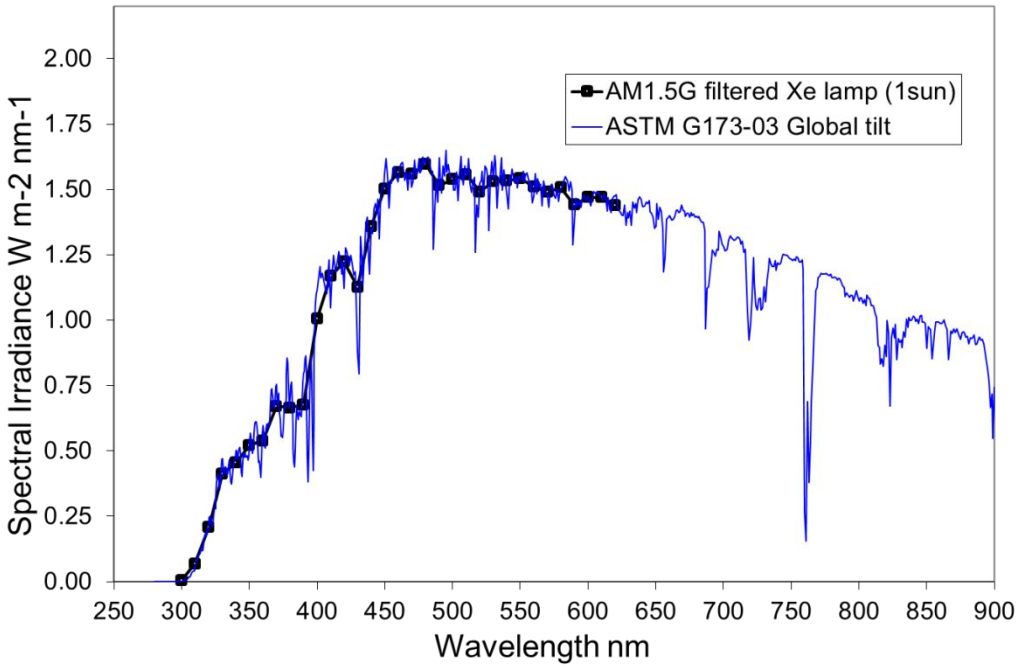

Fig. S1 Spectral data graph for AM 1.5 G filtered 300 W Xe lamp.

Apparent quantum yield calculations

Apparent quantum efficiency (AQE) was measured under the same experimental setup, using 523 nm LED monochromatic light and the equation as follows:

$$\text{AQE} / \% = \frac{\text{Number of reacted electrons}}{\text{Number of incident photons}} \times 100$$

The number of incident photons are calculated using the following equations:

$$\text{Number of moles of incident photons per time } (N_{\text{Einstein}}) = \frac{\text{Number of incident photons per time } (N_p)}{N_A}$$

where N_p can be calculated as follows:

$$N_P = \frac{\text{Light intensity (E)}}{\text{Photon energy } (E_p)} \quad \text{and} \quad \text{photon energy } (E_p) = \frac{hc}{\lambda}; \text{ substituting, we obtain:}$$

$$E_p = \frac{(6.625 \times 10^{-34}\,\text{J s})\,(3 \times 10^{17}\,\text{nm s}^{-1})}{523\,\text{nm}} = 0.038 \times 10^{-17}\text{J};$$

Light intensity (E) = Irradiance (W m^{-2}) $\times$ effective light irradiation area (m^2).

Irradiance in the reactor measured as 9 mW cm^{-2} and the effective light irradiation area was 3.0 cm^2. Therefore, calculated E was 0.027 W or J s^{-1} at 523 nm.

Substituting, we obtain:

$$N_p = \frac{E}{E_p} = \frac{0.027\ J\ s^{-1}}{0.038 \times 10^{-17}\ J} = 0.71 \times 10^{17}\ s^{-1}$$

$$N_{Einstein} = \frac{N_P}{N_A} = \frac{0.71 \times 10^{17}\ s^{-1}}{6.022 \times 10^{23}\ mol^{-1}} = 0.118 \times 10^{-6}\ mol\ s^{-1} = 0.118\ \mu mol\ s^{-1}$$

The production rates of H_2, CO, and CH_4 with 523 nm monochromatic light under given experimental conditions were 0.37, 0.19 and 0.02 µmol h^{-1} respectively. Finally,

$$AQE\ (\%) = \frac{2 \times H2\ production\ rate\ in\ \mu mol\ s^{-1}}{0.118\ \mu mol\ s^{-1}} \times 100 = 0.17$$

$$AQE\ (\%) = \frac{2 \times CO\ production\ rate\ in\ \mu mol\ s^{-1}}{0.118\ \mu mol\ s^{-1}} \times 100 = 0.089$$

$$AQE\ (\%) = \frac{8 \times CO\ production\ rate\ in\ \mu mol\ s^{-1}}{0.118\ \mu mol\ s^{-1}} \times 100 = 0.037$$

Therefore, total AQE in the given experimental condition rGO-MoS_2/PPy-150 nanocomposite is 0.30 %.

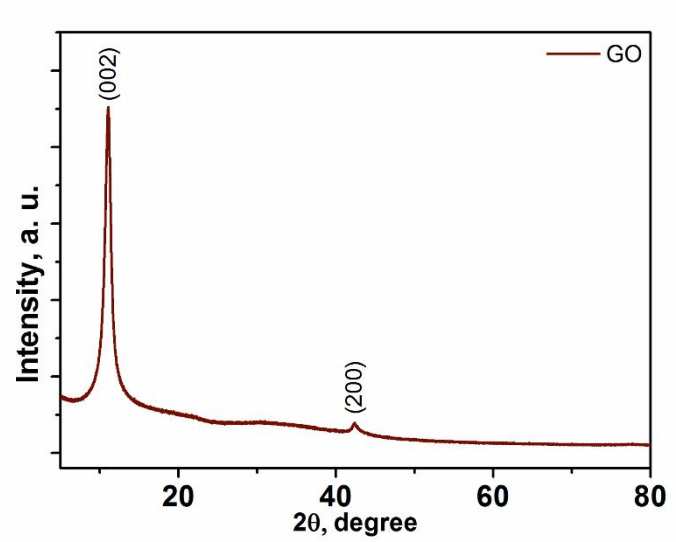

Fig. S2 XRD pattern of graphene oxide (GO).

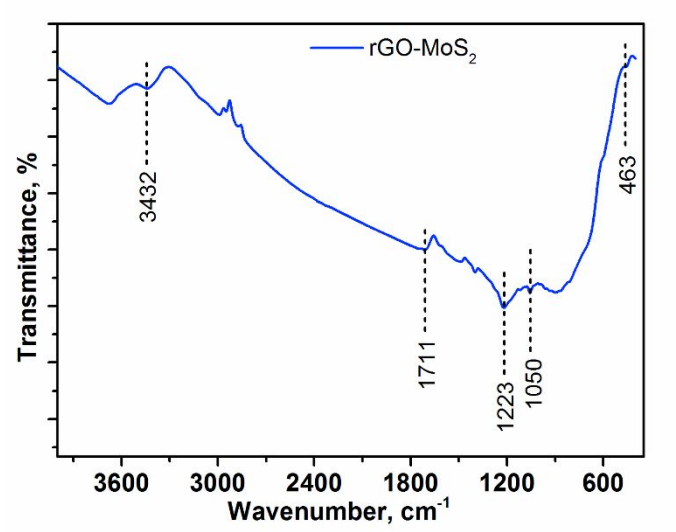

Fig. S3 FTIR spectrum of graphene rGO-MoS_2 nanocomposite.

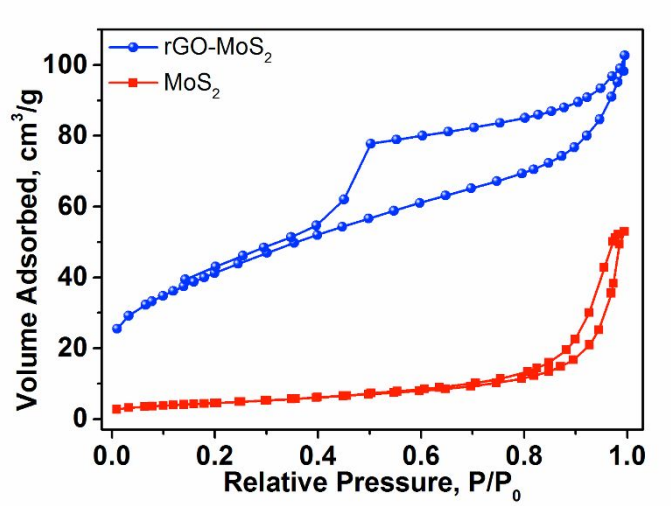

Fig. S4 N_2 adsorption-desorption isotherms of MoS_2 nanosheets and rGO-MoS_2.

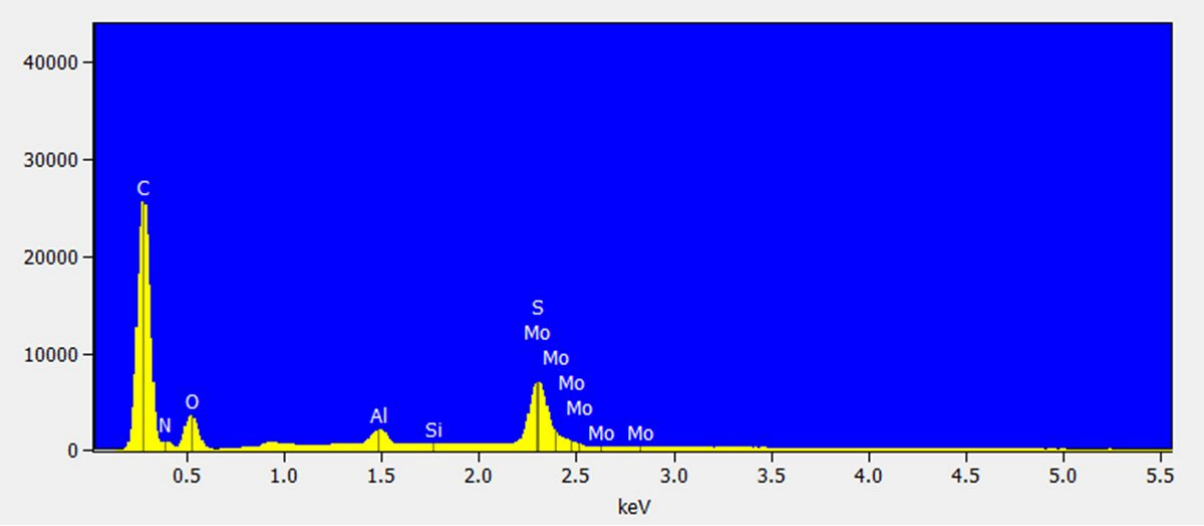

Fig. S5 EDX spectrum of rGO-MoS_2/PPy-150 nanocomposite.

Table S1 BET surface area of MoS_2, rGO-MoS_2, rGO-MoS_2/PPy-600, rGO-MoS_2/PPy-300 and rGO-MoS_2/PPy-150 nanocomposite.

Sample	**Surface Area (S_{BET}), (m^2/g)**
MoS_2	16.1
rGO-MoS_2	149.6
rGO-MoS_2/PPy-600	8.4
rGO-MoS_2/PPy-300	12.5
rGO-MoS_2/PPy-150	16.0

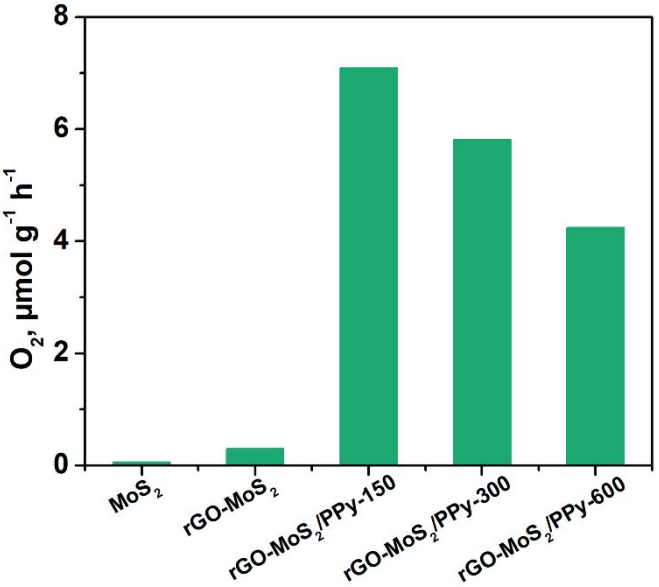

Fig. S6 Rate of O_2 evolution on different photocatalytic systems.

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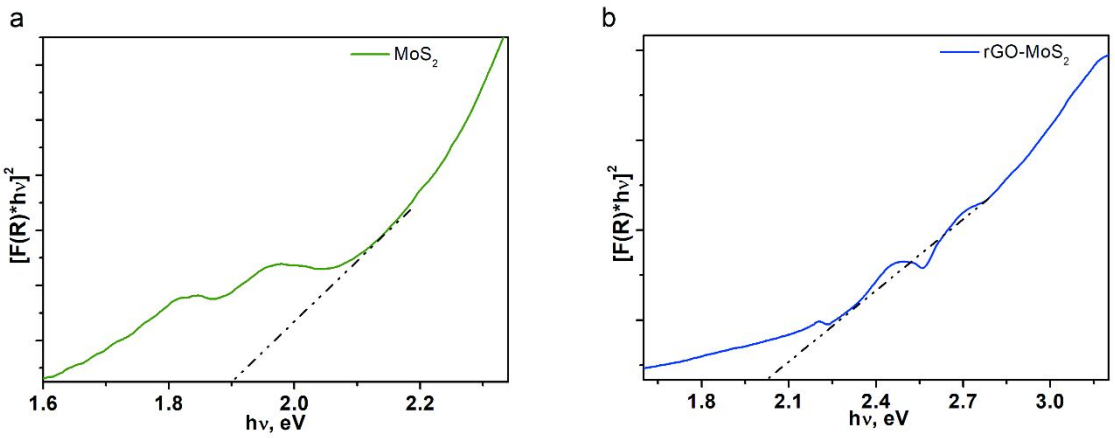

Fig. S7 Tauc's plots of MoS_2 and rGO-MoS_2 for band gap calculation.