SUPPORTING INFORMATION

Supporting Information

Incorporating Au₁₁ Nanocluster on MoS₂ Nanosheet Edges for Promoting

Hydrogen Evolution Reaction at the Interface

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I. Characterizations

(a)



(b)



(c)





Figure S1. (a) PXRD pattern, (b) TEM images and (c) XPS spectra of as-synthesized MoS_2 nanosheets.



Figure S2. (a) Total crystal structure of $Au_{11}(PPh_3)_7I_3$ NC. (Color legends: Au, yellow, blue; P, red; I, green; C, gray; H, orange) and (b) The ultraviolet-visible absorption spectrum of $Au_{11}(PPh_3)_7I_3$ NC in DCM.







(b)





(c)



Figure S3. TEM images and the particle size distribution of the (a) 0.5 % - Au₁₁@MoS₂; (b) 2 % - Au₁₁@MoS₂ and (c) 4 % - Au₁₁@MoS₂ nanocomposites.



Figure S4. XPS spectrum showing absence of ligands in the 2 % - Au₁₁@MoS₂ nanocomposites.



Figure S5: (a-d) is the double layer capacitance in the chosen region of non-Faradaic region for MoS_2 , 0.5 % $-Au_{11}@MoS_2$, 2 % $-Au_{11}@MoS_2$ and 4 % $-Au_{11}@MoS_2$ nanocomposites, respectively.



Figure S6. (a) C_{dl} values of all the three catalyst; (b) bar diagram for the TOF values of different catalyst calculated at 350 mV overpotential; (c) mass activity plot for different catalyst; (d) EASA normalized polarization curve and (e) chronoamperometric outcomes.

II. Post-catalytic Characterizations

(a)



(b)





Figure S7. Post-catalytic characterization: (a) PXRD pattern¹ and (b) XPS spectra of 2 % - Au₁₁@MoS₂ nanocomposite after HER-studies.

III. References

1. Warapa Susingrat, Thapanee Sarakonsri, Nutpaphat Jarulertwathana, Jaroon Jakmunee, Khac Duy Pham and Chung Hoeil, *Journal of Materials Science and Engineering A*, 2017, **7**, 178-187.