Supporting information

Triggering the phase transition of Molybdenum Di-Selenide ($MoSe_2$) 1T@2H by introducing Copper (Cu^+): Experimental Insights and DFT Analysis for hydrogen evolution reaction

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1.Material and reagents

Selenium powder (Se) and Cupric chloride $CuCl_2.2H_2O$ were purchased from Sigma Aldrich and sodium molybdate dihydrate ($Na_2MoO_4.\ 2H_2O$), and hydrazine hydrate solution ($N_2H_4.\ H_2O$) were purchased from Qualigens Fine Chemicals Ltd, sulphuric acid (H_2SO_4; assay 97%), The above chemicals were of analytical grade and used without any further purification.

1.1 Material characterizations

The crystallinity of powdered Pristine $MoSe_2$ and 3% & 5% Cu-$MoSe_2$ samples was examined utilizing a PANalytical EMPYREAN X-ray system with a monochromatic CuKα (λ= 1.5406 Å) radiation source. X-ray photoelectron spectroscopy (XPS) was conducted utilizing the PHI - VERSAPROBE III from Japan to ascertain the elemental makeup and their chemical states. High-resolution scanning electron microscopy (HRSEM) (Thermo-Fisher Scientific, USA) was used to document the morphology of the synthesized Pristine $MoSe_2$, 3% Cu-MoSe2@CC, and 5% Cu-$MoSe_2$@CC samples. The Energy Dispersive X-ray Analysis (EDX) (Oxford instruments) was used to do elemental analysis accompanied by colour mapping.

2. X-ray diffraction patterns (XRD)

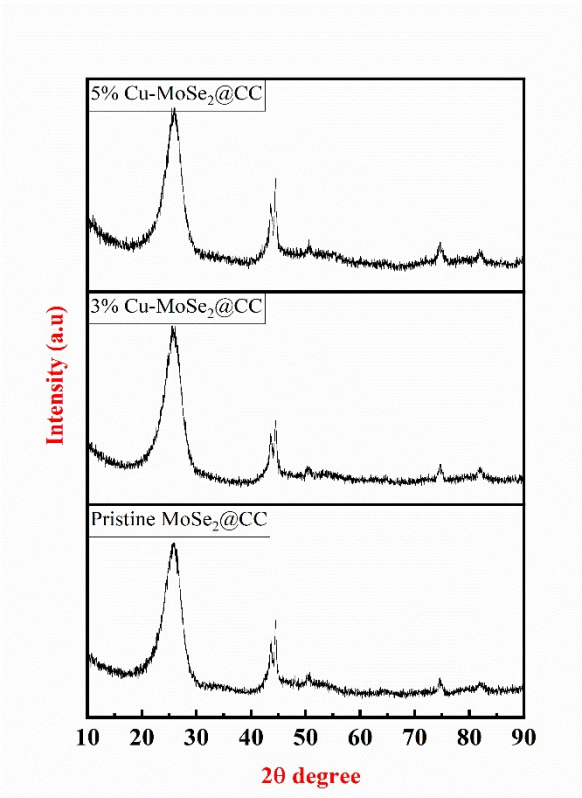

Figure S1- X-ray diffraction patterns of Pristine $MoSe_2$@CC, 3% Cu-$MoSe_2$@CC, and 5% Cu-$MoSe_2$@CC catalyst coated on Carbon cloth

3. X-ray photoelectron spectroscopy (XPS)

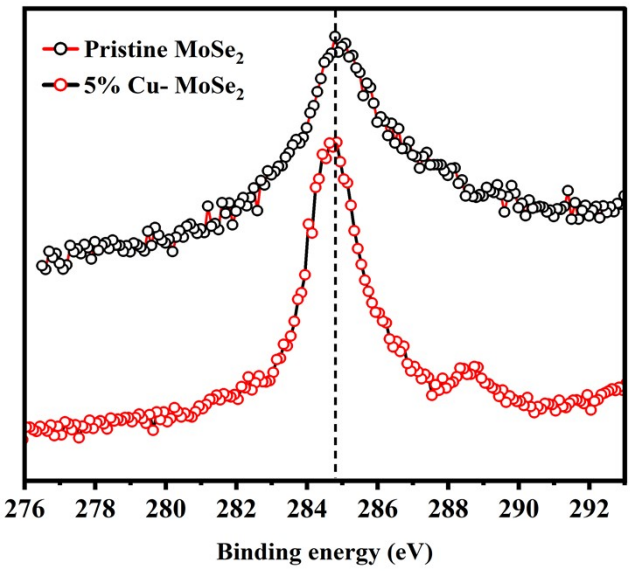

Figure S2 -high resolution XPS spectra of Carbon C1s - samples Pristine $MoSe_2$ and 5%Cu-$MoSe_2$

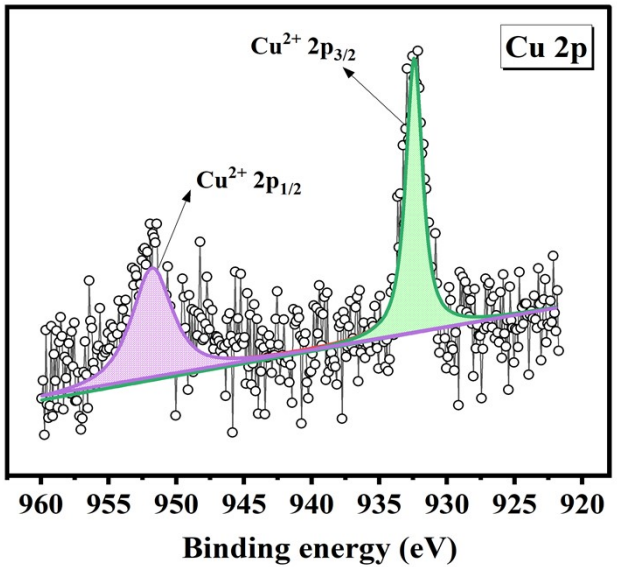

Figure S3- Core-level XPS spectra of Cu-2p

4. Electrochemical activity

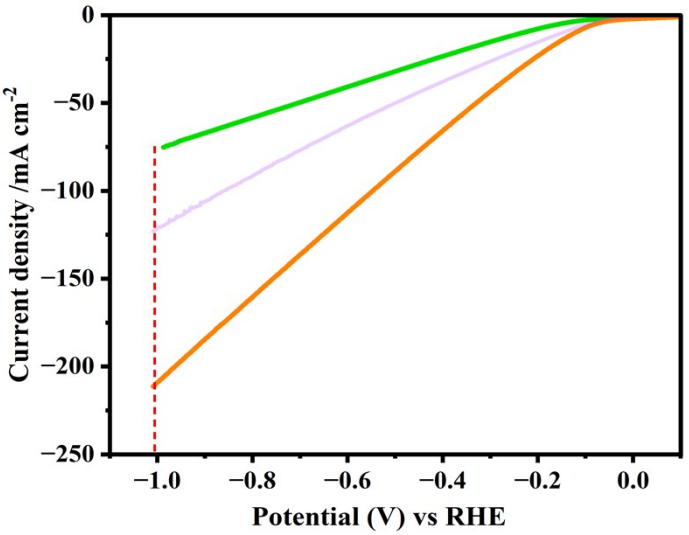

Figure S4-Linear polarization curves indicating the increased current density of adding Cu on $MoSe_2$

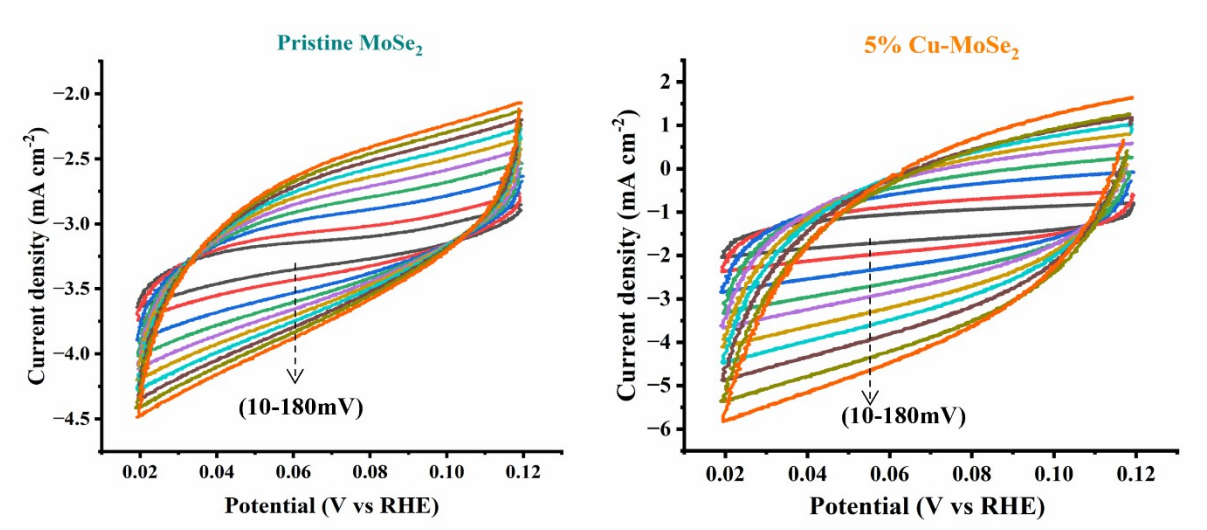

Figure S5 -CV curves between 0.02 and 0.12 of the Pristine $MoSe_2$ & 5%Cu-$MoSe_2$ samples with at different scan rates

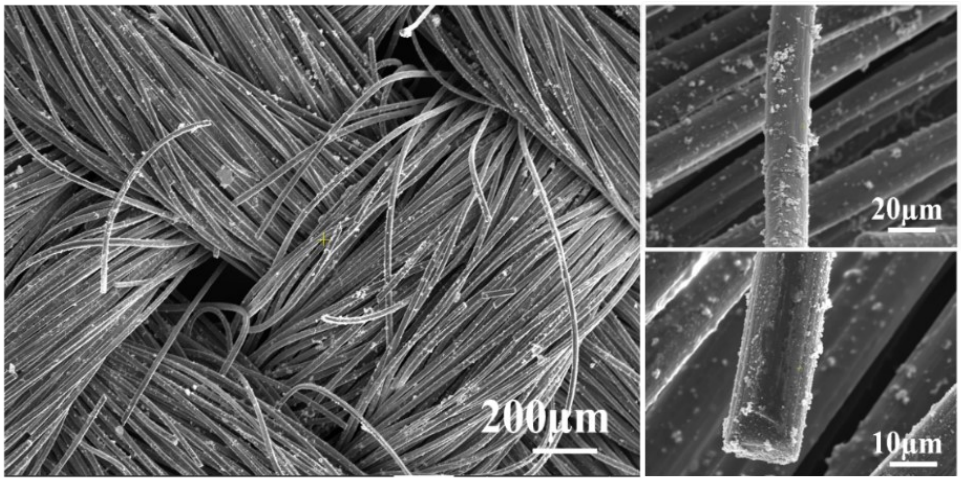

Figure S6 - SEM images with different magnification of after stability of 80hrs

5. DFT

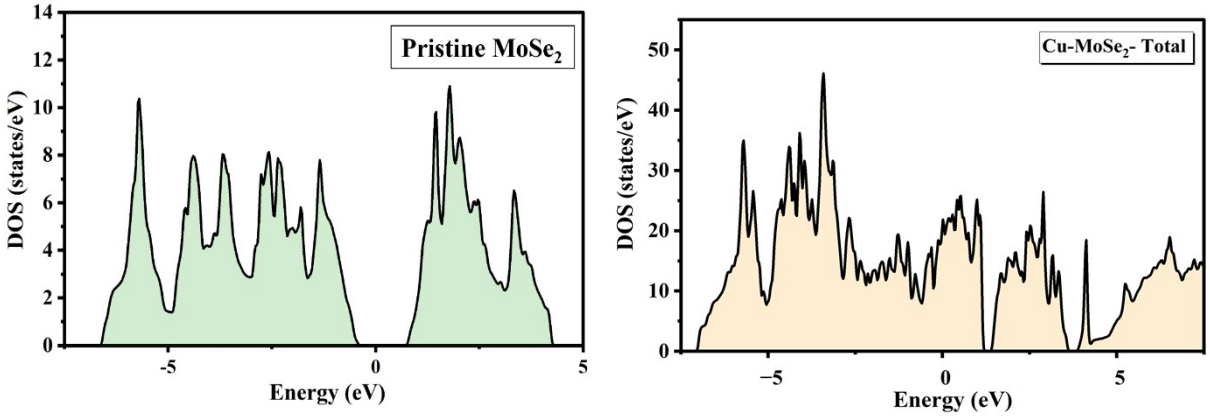

Figure S7 The total density of states as a function of energy for Pristine $MoSe_2$(2H) and Cu-$MoSe_2$(1T)