Electronic Supplementary Information

Snowflake like metastable wurtzite $CuGaS_2/MoS_2$ composite with superior electrochemical HER activity

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We have simulated the diffraction pattern for wurtzite $CuGaS_2$ using the Diamond software and the crystal parameters are given in **Table S1**. The obtained simulated diffraction pattern is shown as the red line pattern in **Figure 1**.

Table S1. Crystal parameters of wurtzite $CuGaS_2$

Atom	Wyck.	x/a	y/b	z/c
Cu	2b	1/3	2/3	0
Ga	2b	1/3	2/3	0
S	2b	1/3	2/3	0.375

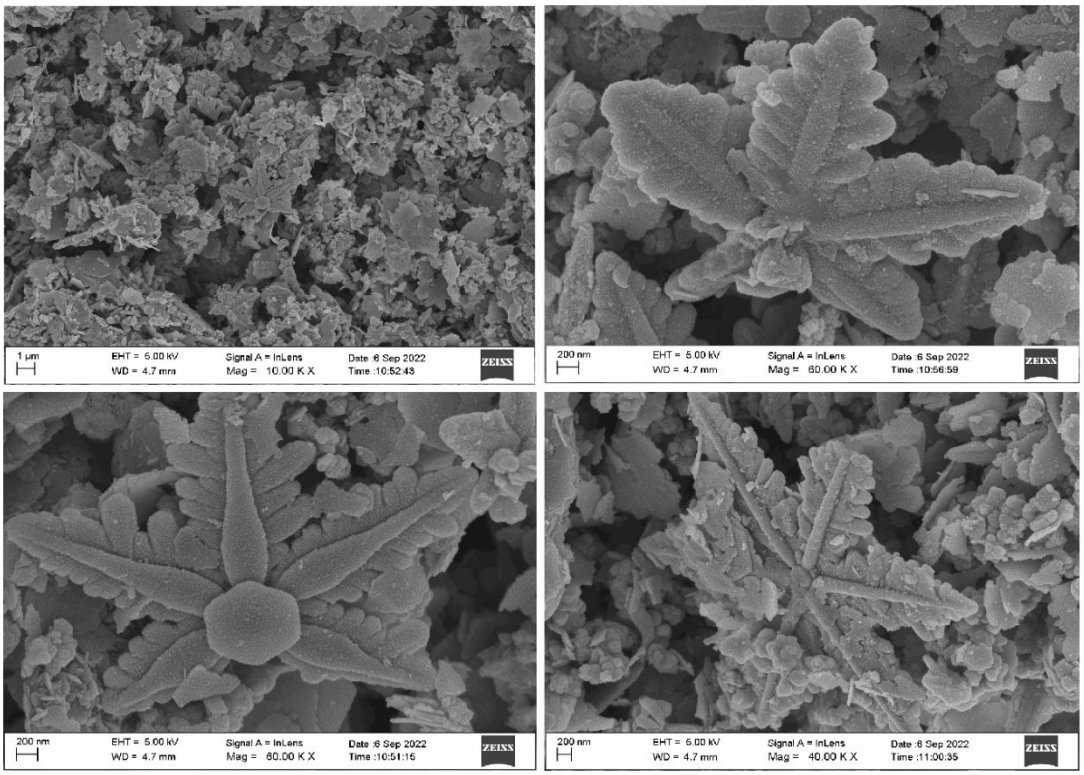

Figure S1. FESEM images of $CuGaS_2$/7%MoS_2 at different magnifications.

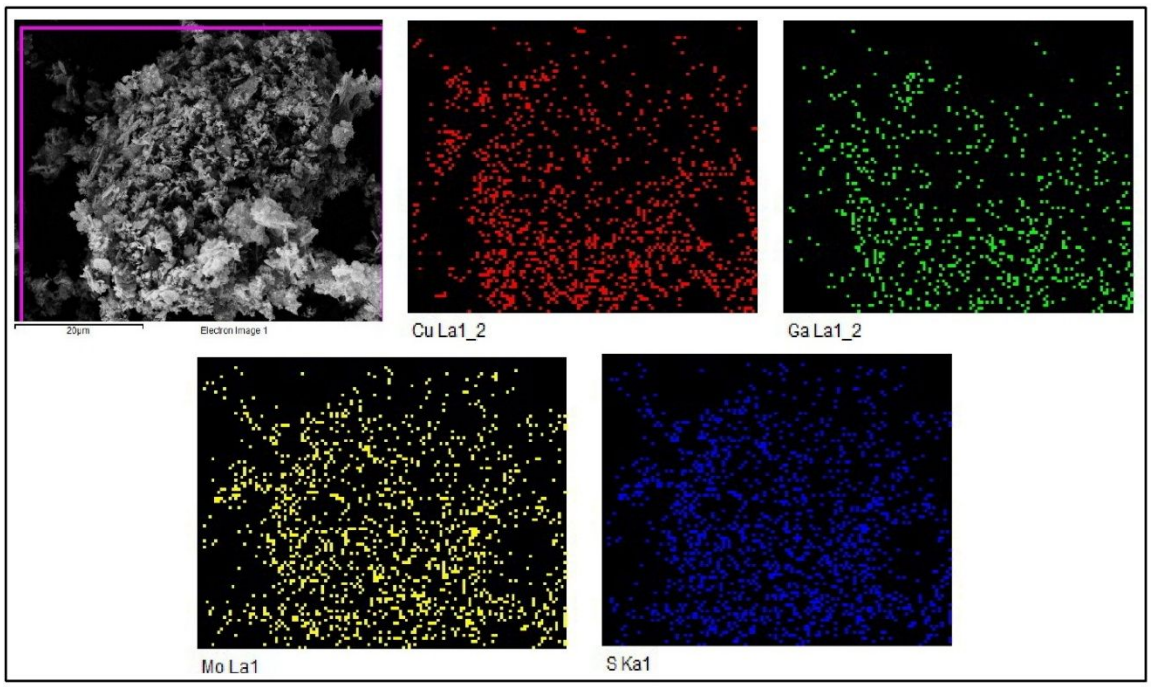

Figure S2. Elemental mapping images of $CuGaS_2$/7%MoS_2 composite.

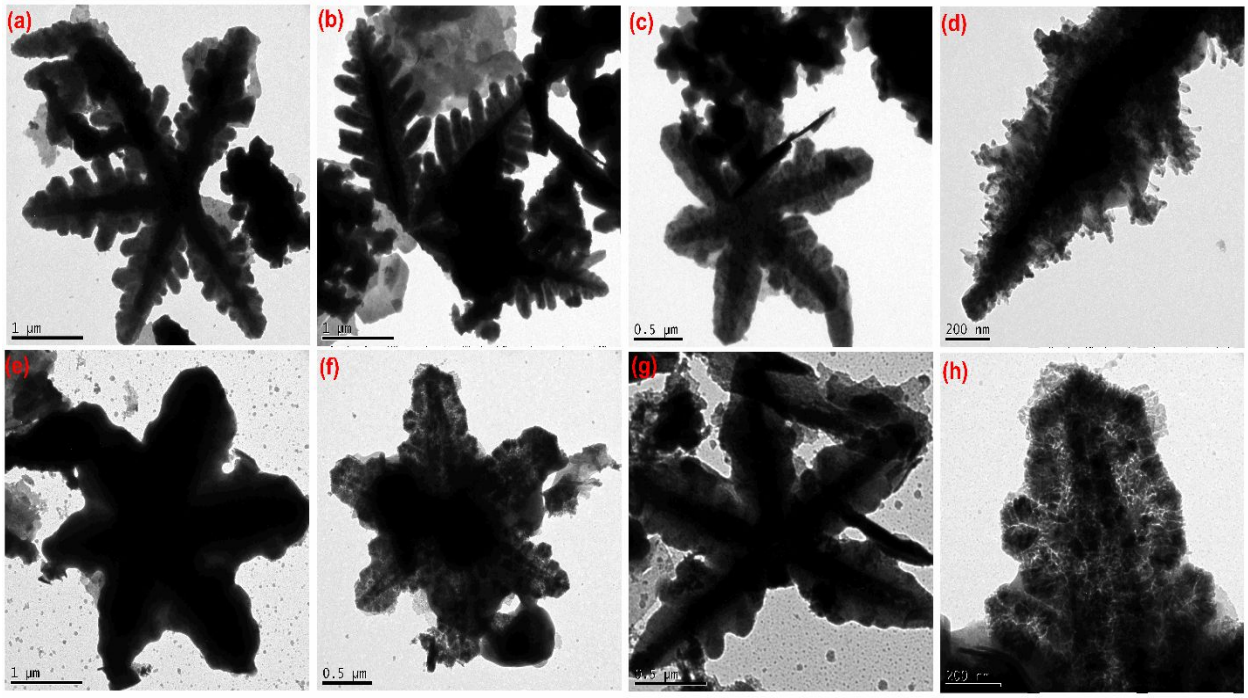

Figure S3. TEM image of $CuGaS_2$ (a, b, c, d) and $CuGaS_2$/7%MoS_2 (e, f, g, h) in different magnifications.

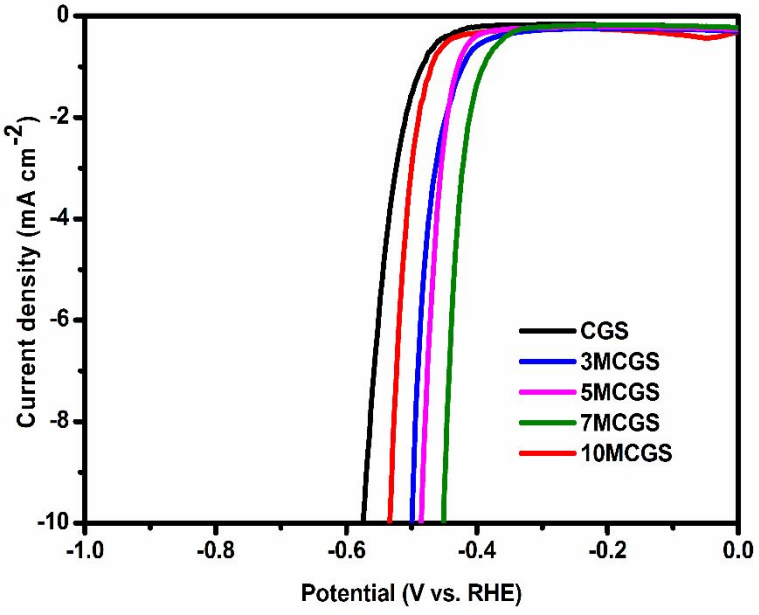

Figure S4. iR-corrected LSV curves of CGS, 3MCGS, 5MCGS, 7MCGS, and 10MCGS for HER in 0.5 M H_2SO_4.

The iR corrected LSV curves shown in **Figure S4** indicate that the catalyst 7MCGS have slightly increased overpotential value (~13 mV) attributed to the iR drop.

Calculation of Electrical double layer capacitance (*Cdl*) and ECSA

Electrochemical active surface area (ECSA) of $CuGaS_2/xMoS_2$ (x=0,3,5,7,10%wt) catalysts was estimated from their electric double layer capacitance (*Cdl*). The double layer capacitance value was measured from the non-Faradaic potential region of the CV curves at different scan rates 50 mV s^{-1} to 10 mV s^{-1} in 0.5 M H_2SO_4. Their anodic and cathodic current densities measured at the middle potential from CV scans were linearly fitted with the CV scan rates to obtain $Slope_{anodic}$ and $Slope_{cathodic}$, respectively.

Cdl was calculated by $Cdl = (Slope_{anodic} - Slope_{cathodic})/2$ --- (1)

ECSA was then calculated by dividing the electric double layer capacitance value (*Cdl)* by the specific surface capacitance (*Cs*) of the electrode surface.

$ECSA = Cdl / Cs$ --- (2)

Since the exact value of *Cs* for $CuGaS_2$ is not available, a commonly used Cs value (0.04 mF cm^{-2}) for metal surfaces was used in this study.[1,2]

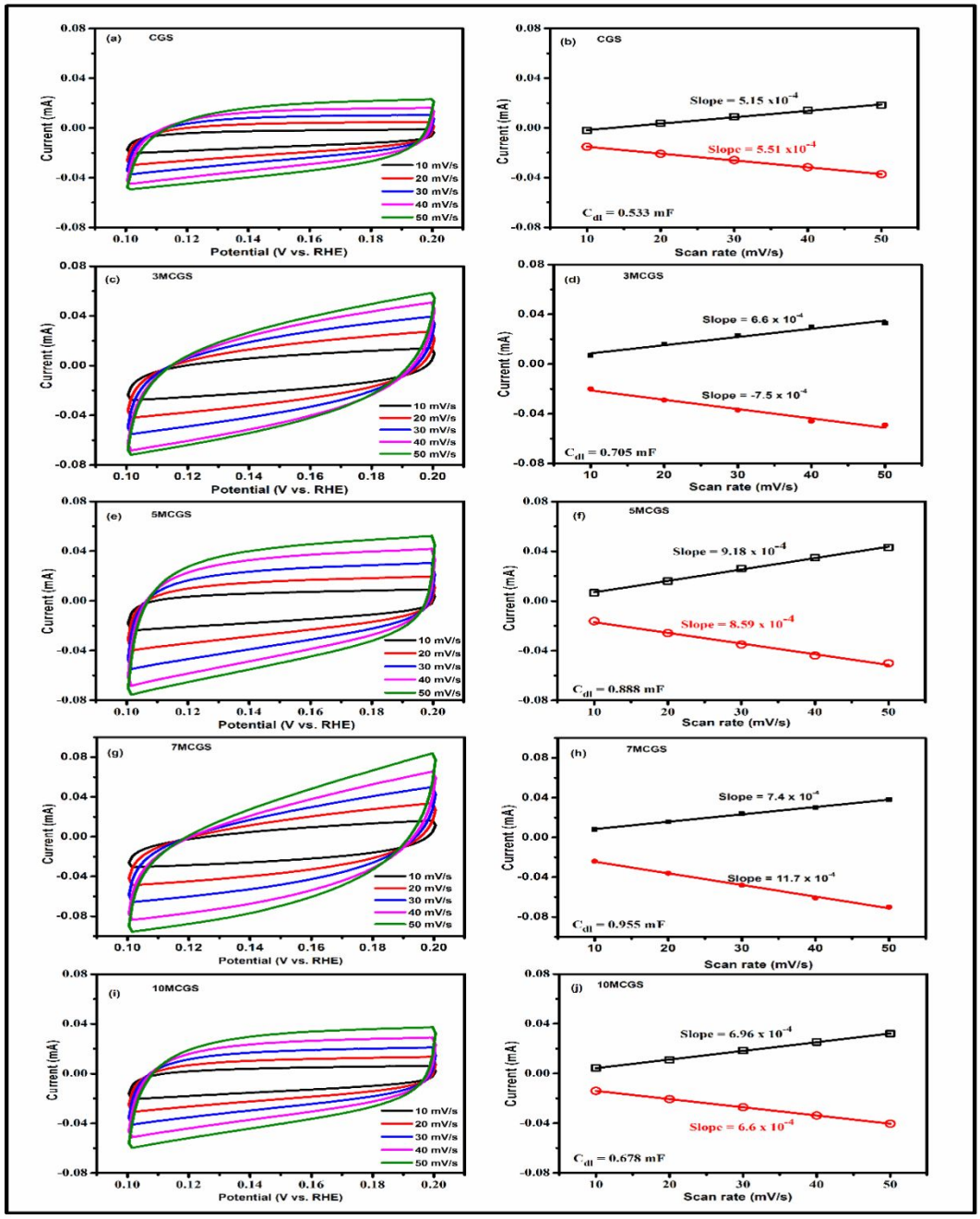

Figure S5. CV curves (a, c, e, g, i) at a non-faradic area in 0.5 M H_2SO_4 at the scan rates of 10, 20, 30, 40 and 50 mV s^{-1} and capacitive currents plotted as a function of the scan rate (b, d, f, h, j) of the CGS, 3MCGS, 5MCGS, 7MCGS, 10MCGS electrodes.

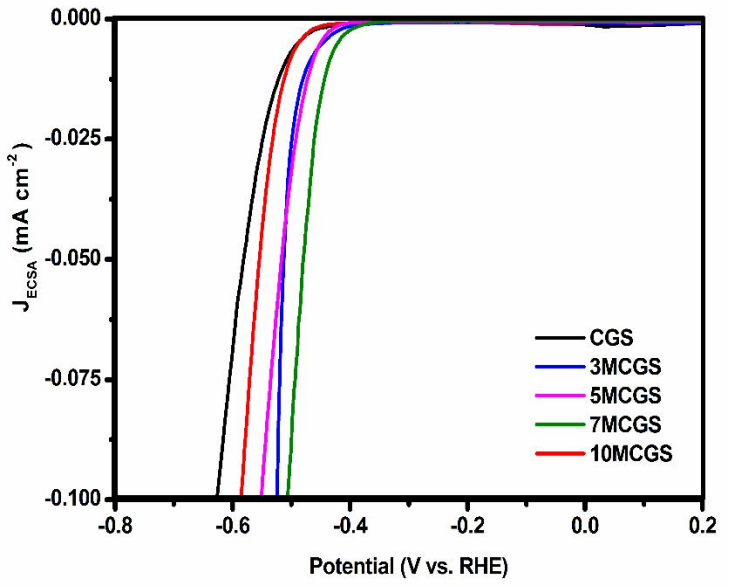

Figure S6. LSV curves of CGS, 3MCGS, 5MCGS, 7MCGS, and 10MCGS normalized by calculated ECSA.

Calculation procedure for TOF:

TOF = JA/2nF

J is current density at particular overpotential in (A cm^{-2}), J at 400 mV

A is surface area of the working electrode (0.07 cm^{-2})

F is Faradays constant value 96485 C/mol

½ is used as HER is a two electron reaction

n is the number of moles of the catalyst loaded on the working electrode

Table S2 Calculated TOF of catalysts

Catalyst	TOF
CGS	4.7×10^{-4}
3MCGS	9.2×10^{-4}
5MCGS	6.2×10^{-4}
7MCGS	19.6×10^{-4}
10MCGS	5.6×10^{-4}

Table S3. Comparison for RhB adsorption performance of different sulfide based adsorbents.

S. No	Adsorbent	Dye concentration (mg/L)	Catalyst amount	Time (min)	Adsorption capacity (mg g^{-1})	Percentage of adsorption	Ref
1	Fe_3O_4/MoS_2 composites	20	20	30	24	-	3
2	SnS_2/MoS_2 NPs	10	20	15	23.6	92	4
3	Flower-like MoS_2 nanostructures	20	20	35	49.2	91	5
4	Ni/MoS_2 nanocomposites	20	10	35	15.7	-	6
5	MoS_2 nanosheets	20	100	5	19.6	97.96	7
6	Flower-like MoS_2 nanostructure	10	10	180	59	98.5	8
7	Snowflake like $CuGaS_2$	10	30	20	15	90	Present study
				60	16.5	99	

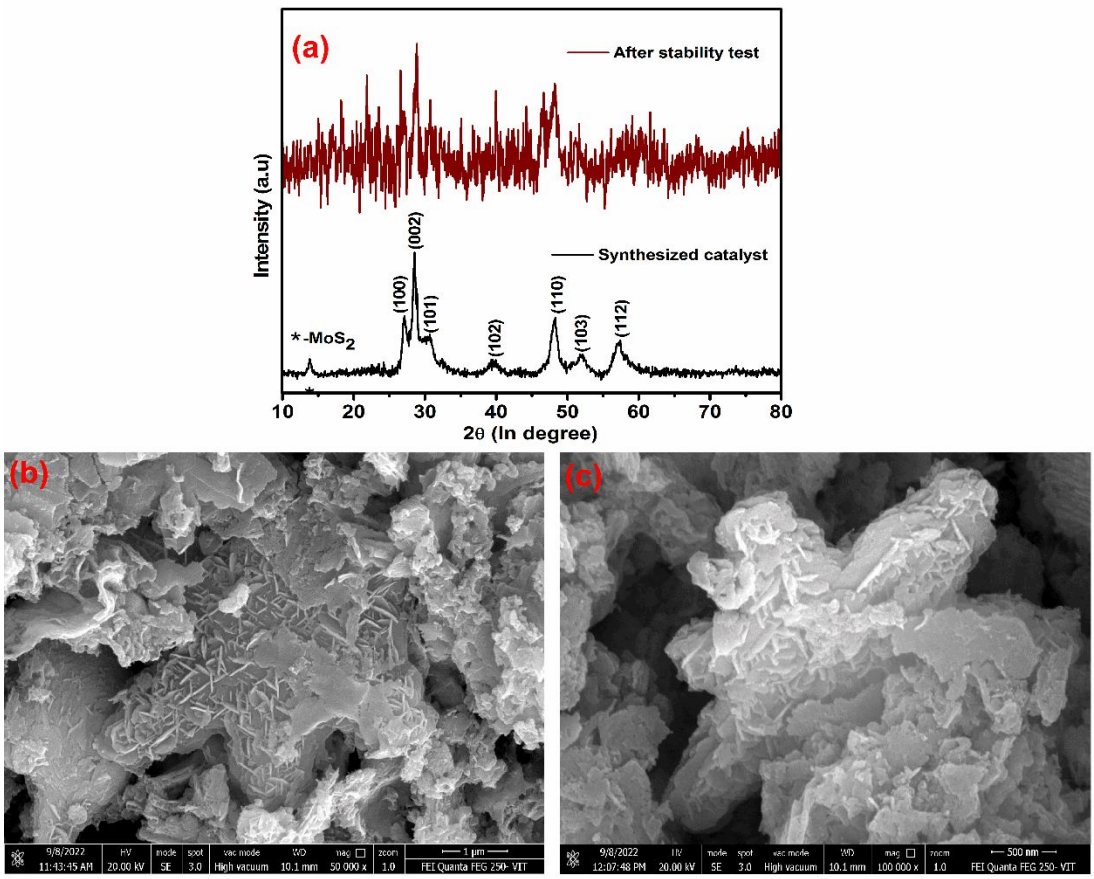

Figure S7. XRD patterns before and after HER activity (a), FESEM (b, c) after HER activity of 7MCGS.

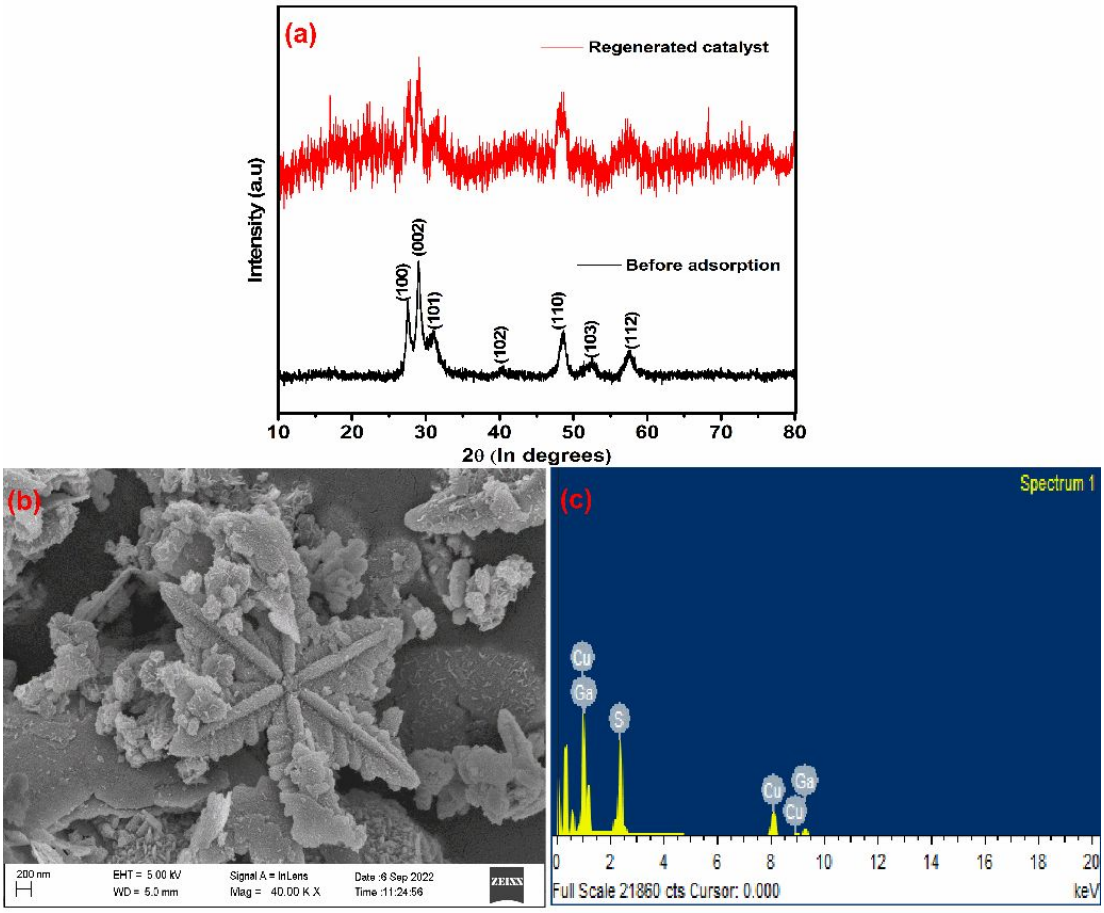

Figure S8. XRD patterns before and after RhB adsorption (a), FESEM image (b) and EDAX (c) after RhB adsorption of $CuGaS_2$.

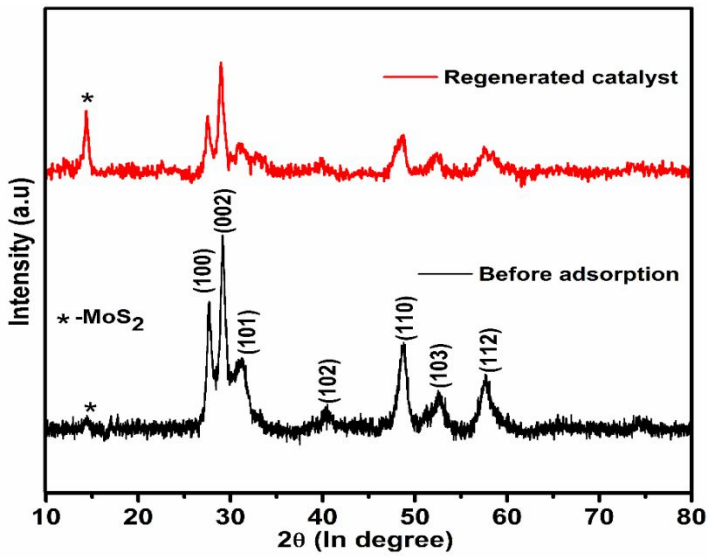

Figure S9. XRD patterns before and after RhB adsorption of $CuGaS_2$/5%MoS_2.

References

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