

High Entropy Alloy Nanoparticles Decorated, p-type 2D-Molybdenum Disulphide (MoS₂) and Gold Schottky Junction Enhanced Hydrogen Sensing

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Supplementary

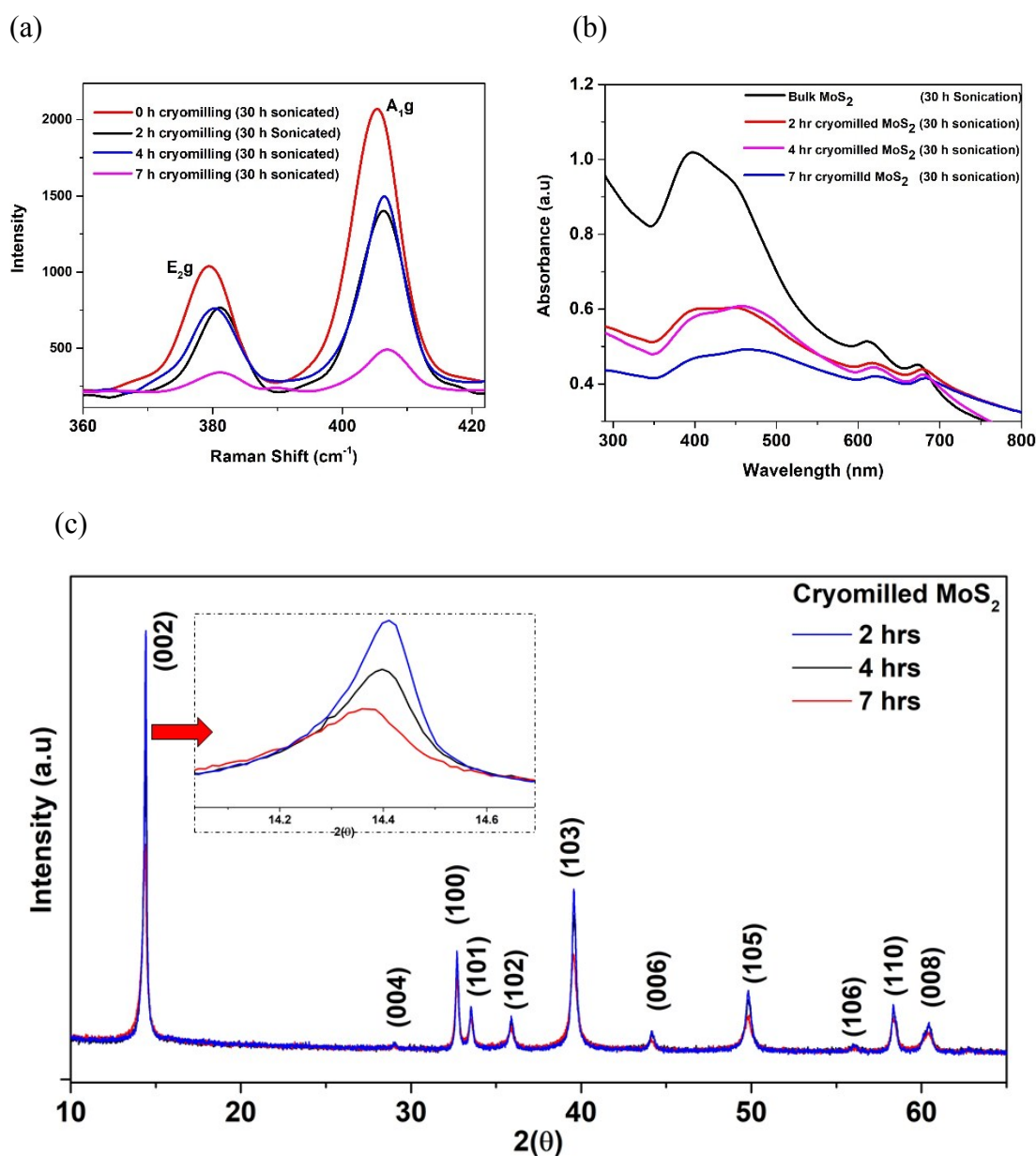
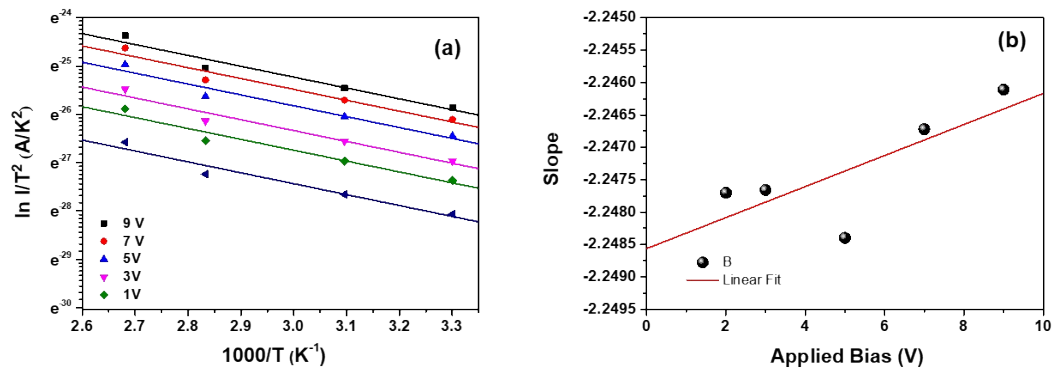


Figure S1: (a) Raman spectrum of successive hours cryomilled and sonicated for 30 hours (b) absorption spectra of MoS₂ in successive hours cryomilling (c) X-ray diffraction pattern of successive hours cryomilling of MoS₂.

Hall Effect:

Hall effect measurement was done at two different values of Magnetic field i.e. 2000 G and 4000 G to confirm the carrier type and it confirms the majority carriers as **p-type**.



Figure

re S2 (a) The variation of I/T^2 Vs $1/T$ at various applied biases and of slope at each bias voltage.

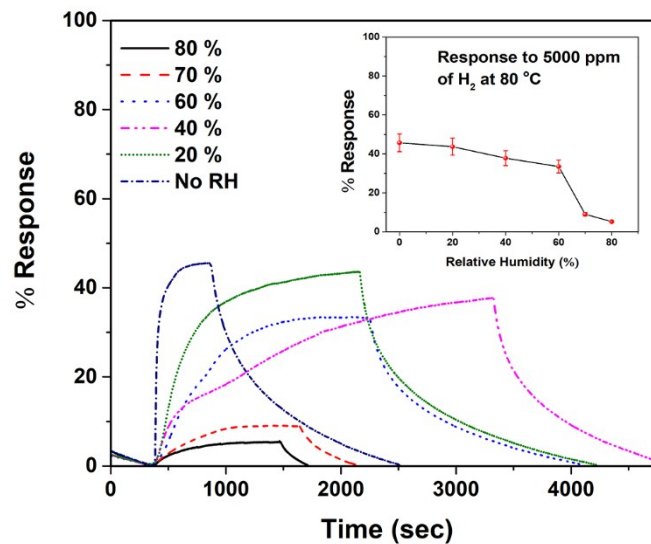


Figure S3. The response of the MoS_2+HEA sample for 5000 ppm of H_2 at $80^\circ C$ for various relative humidity levels.

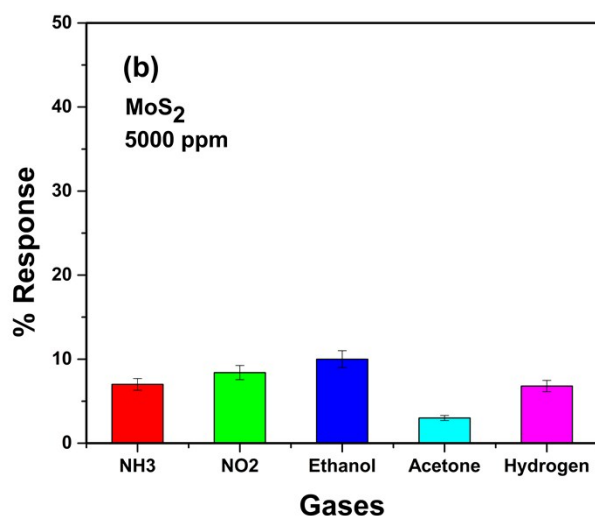


Figure S4: The response of bare MoS₂ sensor towards 5000 ppm of gases at 80°C depicting the cross sensitivity to other gases.

Table S1. The quantification (absolute and relative) of X-ray Photoelectron spectroscopy data.

	MoS ₂				MoS ₂ +HEA			
	BE(eV)	Area	FWHM	Relative	BE(eV)	Area	FWHM	Relative
	(eV)		M	%	(eV)		M	%
S (2S)	226.5	10083.59	1.95		226.9	717.26	2.15	
Mo (+4) 3d 5/2	229.3	41149.91	1.44		229.3	1724.38	1.58	
Mo (+4) 3p 3/2	232.9	17089.00	1.43	67.2	232.3	3823.86	1.66	57.5
Mo (+6) 3d 5/2	232.3	22128.79	1.41		232.9	1245.09	2.10	
Mo (+6) 3p 3/2	235.9	6271.14	1.47	32.8	235.8	2857.87	2.19	42.5
S(-2) 2p 3/2	162.3	15360.79	1.13		162.3	977.62	1.34	
S(-2) 2p 1/2	162.8	7868.44	1.14		163.3	450.50	1.30	
S ₂ (-2) 2p 3/2	163.6	4148.82	0.79		164.1	77.73	0.63	
S ₂ (-2) 2p 1/2	165.0	14479.30	1.88		165.7	235.30	4.64	
SO _x	169.1	248.97	1.02		168.6	1658.37	1.63	
					169.8	853.15	1.71	
O 2s	529.6	52278.54	1.78	55.7	529.5	80744.27	1.70	56.5
O(defect) 2s	531.2	41627.29	2.57	44.3	530.8	62178.21	2.40	43.5

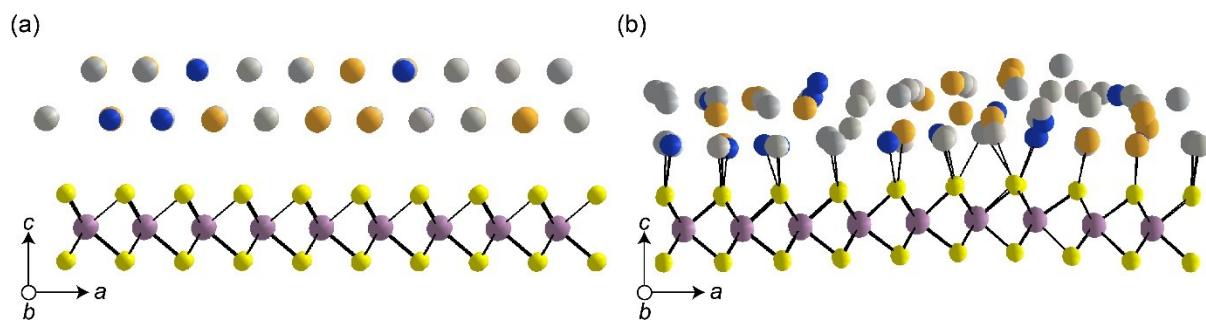


Figure S5. Structures of (a) initial, and (b) completely relaxed MoS₂-HEA system. Light violet, yellow, light grey, dark grey, gold, silver, and blue spheres represent Mo, S, Pt, Pd, Au, Ag, and Cu atoms, respectively.

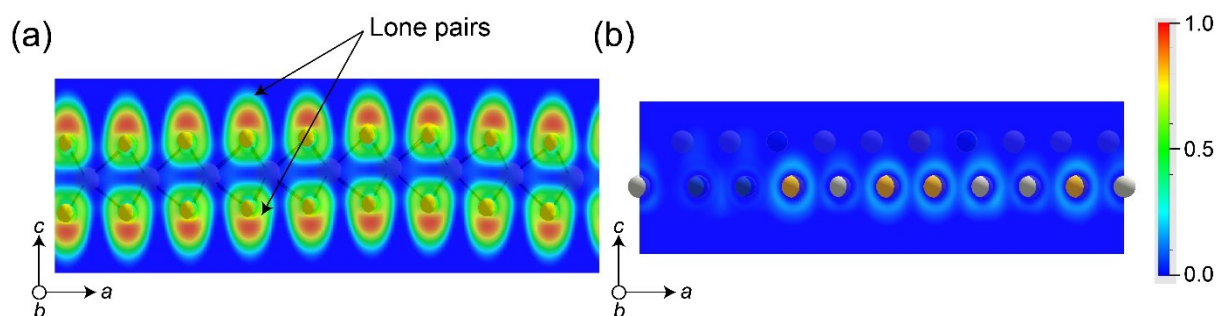


Figure S6. ELF of isolated (a) MoS₂, and (b) HEA systems along (010) plane. The color bar for ELF values are also shown alongside. Violet, yellow, light grey, dark grey, gold, silver, and blue spheres represent Mo, S, Pt, Pd, Au, Ag, and Cu atoms, respectively.

Table S2. DFT energies of completely relaxed structures used in the present study.

System	E_{DFT} (eV)
MoS ₂ (9x4x1 supercell)	- 779.99
PtPdAgAuCu HEA	- 290.56
MoS ₂ + HEA	- 1082.28
H adsorbed on MoS ₂	- 781.57
H adsorbed on MoS ₂ + HEA	- 1086.00
H ₂	- 6.77