Electronic Supplementary Information

Engineering graphene and TMDs based van der Waals heterostructures for photovoltaic and photoelectrochemical solar energy conversion

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Table S1. Selected representative reports of graphene and TMDs based 2D/3D and 2D/2D heterostructure photoelectrodes in PEC cells.

Heterojunction type	Device structure	Photocurrent (mA/cm^2); applied bias	Onset potential (V *vs.* RHE)	Stability (J/J_0); time; applied bias (V *vs.* RHE)	Electrolyte; light source	Ref.
Graphene/semiconductors	F-doped graphene/*n*-Si photoanode	10; 0 V *vs.* E(A/A$^-$)	−0.27 V *vs.* E(A/A$^-$)	~100%; ~28 h; 0 V *vs.* E(A/A$^-$)	50 mM $Fe(CN)_6^{3-}$ and 350 mM $Fe(CN)_6^{4-}$ solution; W-halogen lamp illumination (~33 mW/cm^2)	320
	N-doped monolayer graphene/*p*-Si NW photocathode	−27; 0 V *vs.* RHE	0.35	~30%; ~2.8 h; 0	1 M $HClO_4$ solution (pH = 0); AM 1.5G (100 mW/cm^2)	321
	N-doped graphene quantum sheets/*p*-Si NW photocathode	−35; 0 V *vs.* RHE	0.26	-	1 M $HClO_4$ solution (pH = 0); AM 1.5G (100 mW/cm^2)	322
	$FeNiCoO_x$/graphene micro-net/*n*-Si photoanode	19; 1.5 V *vs.* RHE	1.0	~71%; 1 h; 1.5	1 M NaOH solution (pH = 14); AM 1.5G (100 mW/cm^2)	325
	Graphene/Cu_2O photocathode	−4.8; 0 V *vs.* RHE	0.6	~83.3%; 20 min; 0	Na_2SO_4 with 1.0 M buffer solution (pH = 5); AM 1.5G (100 mW/cm^2)	326
	$BiV_{1-x}Mo_xO_4$/graphene/*α*-Fe_2O_3 photoanode	1.97; 1.6 V *vs.* RHE	0.27	~100%; 12 h; 1.2	0.01 M Na_2SO_4 solution; AM 1.5G (100 mW/cm^2)	332
	NiFe-LDH/graphene/TiO_2 photoanode	1.74; 1.25 V *vs.* SCE	0.35	~100%; 5 h; 0.6 V *vs.* SCE	0.5 M Na_2SO_4 solution (pH = 6.8); Xe lamp (100 mW/cm^2)	334
	MoS_2/N-graphene/g-C_3N_4 photoanode	27.76 μA cm^{-2} at 0.8 V *vs.* Ag/AgCl	-	~100%; ~24 min; 0 V *vs.* Ag/AgCl	0.01 M Na_2SO_4 solution (pH = 7); AM 1.5G (100 mW/cm^2)	336
	p-Cu_2O/graphene photocathode (CO_2 reduction)	−0.75; 0.05 V *vs.* Ag/AgCl	-	~100%; 6 h; −0.05 and +0.05 V *vs.* Ag/AgCl	Phosphate buffer solution (pH = 4.0); AM 1.5G with a UV-cutoff filter	344
	FTO/f-RGO/rr-P3HT:PCBM/TiO_2/Pt photocathode	−6.01; 0 V *vs.* RHE	0.6	~57%; 20 h; 0	Sodium acetate/acetic acid buffer (pH = 4); AM 1.5G (100 mW/cm^2)	345
TMDs/semiconductors	Mo_3S_4/*p*-Si pillars photocathode	−8; 0 V *vs.* RHE	0.15	~100%; 1 h; 0	1 M $HClO_4$ (pH = 0); AM 1.5G (>620 nm, 28.3 mW/cm^2)	347

MoS_3/*p*-InP pillars photocathode	−21; 0 V *vs.* RHE	0.6	~100%; 1 h; 0	1 M $HClO_4$; AM 1.5G (100 mW/cm^2)	348
MoS_x/*p*-GaP photocathode	−6.4; 0 V *vs.* RHE	0.71	~100%; 5 h; 0	1 M $HClO_4$ (pH = 0); AM 1.5G (100 mW/cm^2)	349
MoS_2/*p*-Si NW photocathode	−1; 0 V *vs.* RHE	0.25	~100%; 1 h; −0.1	Na_2SO_4 with 1.0 M buffer solution (pH = 5); Xe lamp with a 420 nm cut-off filter (100 mW/cm^2)	350
MoS_x/Ti/n$^+$p-Si photocathode	−16; 0 V *vs.* RHE	0.33	~100%; 1 h; 0.2	1 M $HClO_4$; AM 1.5 G (>635 nm, 38.6 mW/cm^2)	351
MoS_2/TiO_2/Si photocathode	−15; 0 V *vs.* RHE	0.30	~100%; 1.25 h; –0.33	0.5 M H_2SO_4 (pH = 0.48); AM 1.5G (100 mW/cm^2)	353
MoS_2/Al_2O_3/n$^+$p Si photocathode	−32; 0 V *vs.* RHE	0.4	~100%; 120 h; 0	1 M $HClO_4$ (pH = 0); AM 1.5G (100 mW/cm^2)	355
MoS_x/MoS_2/Mo/n$^+$ p-Si photocathode	-12; 0 V *vs.* RHE	0.334	~100%; 120 h; 0	1 M $HClO_4$; AM 1.5 G (>635 nm, 39.5 mW/cm^2)	356
Mo_3S_{13}/MoS_2/Mo/ Mo_xSi/n$^+$p-Si photocathode	−17.5; 0 V *vs.* RHE	0.40	~100%; 100 h; 0	0.5 M H_2SO_4; AM 1.5G (100 mW/cm^2)	357
MoS_2/MoO_x/SiO_2/ $MoSi_x$/Si photocathode	−18.5; 0 V *vs.* RHE	0.31	~100%; 1538 h; 0	0.5 M H_2SO_4; AM 1.5G (100 mW/cm^2)	358
MoS_2/Mo/$GaInP_2$ photocathode	−6; 0 V *vs.* RHE	0.36	~100%; 70 h; –0.025	3 M H_2SO_4; AM 1.5G (100 mW/cm^2)	359
MoS_2/*p*-Si photocathode	−21.4; 0 V *vs.* RHE	0.23	~100%; 24 h; –0.29	0.5 M H_2SO_4 (pH = 0.3); AM 1.5G (100 mW/cm^2)	361
MoS_2 (13 nm)/*p*-Si photocathode	−24.6; 0 V *vs.* RHE	0.17	~100%; 50 h; 0	0.5 M H_2SO_4 (pH = 1.1); AM 1.5G (100 mW/cm^2)	362
WS_2 (23 nm)/*p*-Si photocathode	−8.3; 0 V *vs.* RHE	0.2	~83%; 10 h; 0	0.5 M H_2SO_4 (pH = 0.27); AM 1.5G (100 mW/cm^2)	364
1T-MoS_2/*p*-Si photocathode	−17.6; 0 V *vs.* RHE	0.25	~77%; 3 h; 0	0.5 M H_2SO_4; AM 1.5G (100 mW/cm^2)	366
MoS_xCl_y/*p*-Si photocathode	−20.6; 0 V *vs.* RHE	0.27	-	0.5 M H_2SO_4 (pH = 0.16); AM 1.5G (100 mW/cm^2)	367
MoS_xCl_y/*p*-Si micro-pyramids photocathode	−43.0; 0 V *vs.* RHE	0.41	~100%; 2 h; 0	0.5 M H_2SO_4; AM 1.5G (100 mW/cm^2)	368

	$MoSe_xCl_y$/*p*-Si micro-pyramids photocathode	−38.8; 0 V *vs.* RHE	0.35	~100%; 2 h; 0	0.5 M H_2SO_4; AM 1.5G (100 mW/cm^2)	368
	a-$CoMoS_x$/Si photocathode	–17.5; 0 V *vs.* RHE	0.25	~93%; ~3.2 h; 0	Phosphate electrolyte (pH = 4.25); AM 1.5G (100 mW/cm^2)	370
	$CoMoS_x$/*p*-Si microwire photocathode	–17.2; 0 V *vs.* RHE	0.192	~67%; 8 h; 0	0.5 M H_2SO_4 (pH = 0.3); AM 1.5G (100 mW/cm^2)	371
	MoO_xS_y/*p*-Si microwire photocathode	–9.83; 0 V *vs.* RHE	0.24	~100%; 2 h; 0	0.5 M K_2SO_4 solution (pH = 1); AM 1.5G (IR filtered; 60 mW/cm^2)	372
	S:MoP/*p*-Si photocathode	–33.1; 0 V *vs.* RHE	0.28	~80%; 2.8 h; 0	0.5 M H_2SO_4 (pH = 1.1); AM 1.5G (100 mW/cm^2)	373
	MoS_{2-x}/TiO_2/AZO/*p*-Cu_2O photocathode	–5.7; 0 V *vs.* RHE	0.45	~100%; 5 h at pH = 1, 10 h at pH = 4 or 9; 0	0.5 M Na_2SO_4 with 0.2 M potassium hydrogen phthalate buffer; AM 1.5G (100 mW/cm^2)	316
Ultrathin TMDs photoeletrodes	WSe_2 nanoflake photocathode (~25 nm)	–1.0; 0 V *vs.* RHE	0.5	~100%; 27 min; 0	1 M H_2SO_4 solution (pH = 0); AM 1.5G (100 mW/cm^2)	423
	Edge-passivated WSe_2 nanoflake photocathode (~18 nm)	-2.64; −0.37 V vs. Ag/AgCl	−0.2 V *vs.* Ag/AgCl	-	Chloranil in MeCN; AM 1.5G (100 mW/cm^2)	424
	Pre-annealed, HTS-passivated WSe_2 nanoflake photocathode (~11 nm)	~-4; 0 V *vs.* RHE	0.4	~100%; > 2 h; 0	1 M H_2SO_4 solution (pH = 0); AM 1.5G (100 mW/cm^2)	448
	MoS_2/perylene-diimide (PDI) photoanode (~10 nm)	~2.60; 0.1 V *vs.* Ag/AgCl	−0.3 V *vs.* Ag/AgCl	~100%; 300 s; 0.1 V *vs.* Ag/AgCl	25 mM LiI in 0.1 M TBAP acetonitrile solution; AM 1.5G (100 mW/cm^2)	426
	MoS_2/WS_2 photoanode (~60 nm)	0.45; 1.23 V *vs.* RHE	0.6	~100%; 1 h; 1	0.5 M $NaClO_4$ solution (pH = 1); AM 1.5G (100 mW/cm^2)	427
	$ZnIn_2S_4$/$MoSe_2$ photoanode	−6.8; −0.8 V *vs.* SCE	−0.35 V *vs.* SCE	~87%; ~280 s; -	0.2 M Na_2SO_4 (pH = 6.8 ; Xe lamp (λ>400 nm)	417
	Black phosphorus/WS_2 photocathode	−2.25; −1 V *vs.* Ag/AgCl	−0.61 V *vs.* Ag/AgCl	~91%; ~240 s; 0.3 V *vs.* Ag/AgCl	0.1 M NaOH ethanol solution; Xe lamp (>780 nm irradiation)	461