

Self-assembled MoS₂/rGO Nanocomposites with Tunable UV-IR Absorption

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Figure S1 shows the SEM images of MoS₂/rGO composites on a SiO₂/Si substrate after annealing for the different TAA/GO ratios: (a) 1:0, (b) 1:1, (c) 1:2 and (d) 1:3. rGO deriving from GO acts as a dispersing platform, efficiently reducing the aggregation of MoS₂ with a decrease of the TAA/GO ratio and forming self-assembled layered MoS₂/rGO structures during the hydrothermal process. The morphology of the annealed structure is slightly different from the morphology of as-grown structure (Fig. 1).

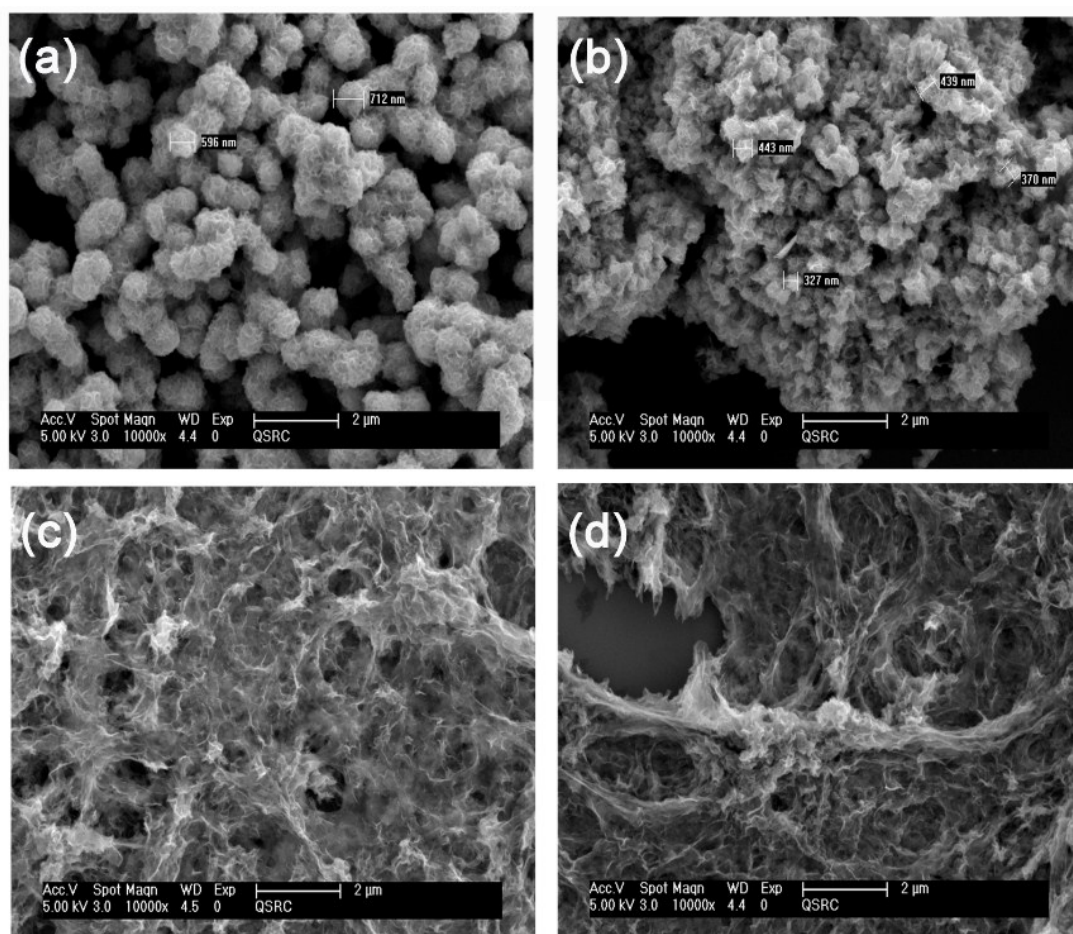


Figure S1. SEM images of MoS₂/rGO composites on a SiO₂/Si substrate after annealing for the different TAA/GO ratios: (a) 1:0, (b) 1:1, (c) 1:2 and (d) 1:3.

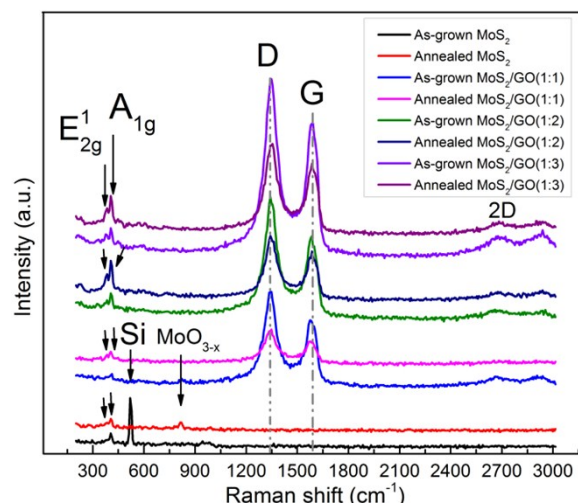


Figure S2. Raman spectra of MoS₂ and MoS₂/rGO composites with different GO content before and after annealing (fitted with Lorentzian functions).

The Raman spectra of MoS₂ (Fig. S2) show the weak peak at 820 cm⁻¹ which corresponds to the M=O bending stretch vibrations for MoO_{3-x} and can be ascribed to the formation of molybdenum oxide during annealing process [1-2]. This peak disappears in the spectra of MoS₂/GO composites, indicating a stronger binding of oxygen to carbon. The origin of the main peaks of the MoS₂/r-GO composite (E¹_{2g}, A_{1g} and G, D) is discussed in the description of Fig. 2b. The 520 cm⁻¹ peak and the peaks at ~2700 and ~2930 cm⁻¹ correspond to the Si substrate [3] and the second-order 2D and D+G bands of graphene [4-5], respectively.

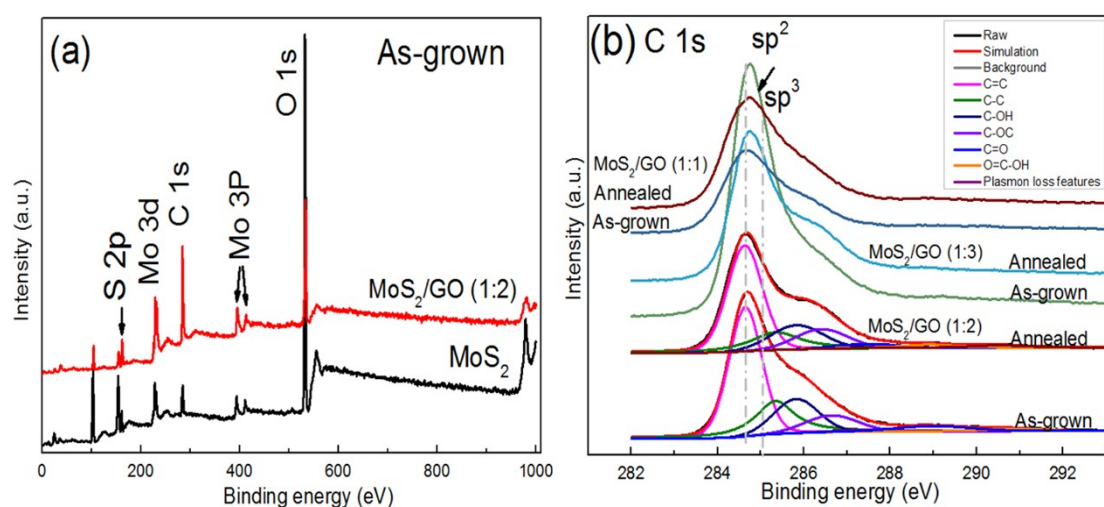


Figure S3. X-ray photoelectron spectra of MoS₂ and MoS₂/rGO composites corresponding to (a) survey, and (b) C 1s core levels.

The chemical composition and binding energies of elements in MoS₂/rGO composites were investigated using XPS. Figure S3 shows the X-ray photoelectron spectra of MoS₂ and MoS₂/rGO composites corresponding to (a) survey, and (b) C 1s core levels. To fit the spectra of composites with MoS₂/GO ratios 1:2 and 1:3, two doublets and splittings of 1.2 and 3.1 eV for S 2p and Mo 3d, respectively, were used. The stronger C 1s signal of the MoS₂/GO (1:2) compared to MoS₂ (Fig. S3a) clearly indicates a significant hydrothermal GO reduction during the synthesis. The low intensity of the Mo 3d signals is apparently due to the formation of Mo₂S_xO_{1-x} and Mo₂S₅, which shows an intermediate product in the MoS₃-to-MoS₂ transition reacting with oxygen from GO deoxygenation. The spectra of C 1s can be decomposed into six components. Peaks at 284.6, 285.3, 285.8, 286.6, 287.5, 288.99 correspond to C=C (sp²) of 48.1 %, C-C (sp³) of 20.4 %, C-OH of 16.4 %, C-O-C of 9.5 %, C=O of 1.2 %, and O=C-OH of 4.4 %, respectively, further confirming the existence of rGO in the composites (Fig. S3b).

Table S1. Detailed characteristics of Raman scattering of MoS₂ and MoS₂/rGO composites.

Specimen		Peak position(cm ⁻¹)		FWHM (cm ⁻¹)		Peak position(cm ⁻¹)	
		E ¹ _{2g}	A _{1g}	E ¹ _{2g}	A _{1g}	D	G
MoS ₂	As-grown	381.2	407.6	35.1	12.8	/	/
	Annealed	381.2	407.4	26.96	12.7	/	/
MoS ₂ /rGO (1:1)	As-grown	381.9	406.6	30.6	19.9	1342.3	1576.4
	Annealed	382.1	405.3	28.4	17.6	1341.7	1573.98
MoS ₂ /rGO (1:2)	As-grown	382.1	404.6	22.0	13.6	1345.9	1578.6
	Annealed	382.6	404.5	21.3	15.7	1348.7	1581.4
MoS ₂ /rGO (1:3)	As-grown	382.6	404.4	17.9	12.1	1347.6	1581.7
	Annealed	382.7	404.1	20.5	15.2	1349.1	1581.9

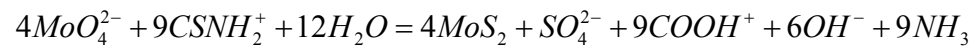
Table S2. Chemical composition and energy of chemical bonds of components.

Specimen		Chemical Composition (At. %)		Mo 3d _{5/2} (eV)			S 2p _{3/2} (eV)	
		S	Mo	S-Mo-S	S-Mo-O	O-Mo-O	S-Mo-S	S-Mo-O
MoS ₂	As-grown	59.8	40.2	229.4	229.7	233.4	161.4	162.2
	Annealed	67.97	32.1	229.5	230.4	233.3	161.6	162.3
MoS ₂ /rGO (1:1)	As-grown	58.5	41.5	229.2	229.6	232.6	162.1	162.2
	Annealed	60.3	39.7	229.2	229.7	232.9	162.0	162.4
MoS ₂ /rGO (1:2)	As-grown	59.8	40.2	229.4	230.6	232.8	162.2	162.7
	Annealed	61.6	38.4	229.3	229.8	232.8	162.1	162.5
MoS ₂ /rGO (1:3)	As-grown	56.9	43.1	229.5	229.8	232.7	162.3	162.6
	Annealed	64.7	35.3	229.5	231.6	233.2	162.2	162.6

Table S3. Detailed C1s bonds for the MoS₂/rGO (1:2) composite.

Specimen		As-grown MoS ₂ /rGO (1:2)		Annealed MoS ₂ /rGO (1:2)	
		Energy (eV)	At.%	Energy (eV)	At.%
Bonding	C=C (sp ²)	284.6	48.1	284.6	48.8
	C-C (sp ³)	285.3	20.4	285.4	15.9
	C-OH	285.8	16.4	285.8	15.8
	C-O-C	286.6	9.5	286.4	12.9
	C=O	287.5	1.2	287.5	3.3
	O=C-OH	289	4.4	288.9	3.3
	Plasmon loss feature	290.9	/	290.5	/

The chemical reaction for the hydrothermal synthesis can be described as:



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