Strains Induced Magnetic Hysteresis in MoS2 and WS2 Monolayers

with Symmetric Double Sulfur Vacancy Defects

LinXue,[a,d] Chaoyu He,[b] Zhi Yang,[a] Zhiyi Zhang,[c] Lichun Xu, [a] Xiaopeng Fan,[a] LonglongZhang,[*a] and Lingzhen Yang[*a]

[a]College of Physics and Optoelectronics, Taiyuan University of Technology, Taiyuan, 030024, China. E-mail: yanglingzhen@tyut.edu.cn; zhanglonglong@tyut.edu.cn

[b]Laboratory for Quantum Engineering and Micro-Nano Energy Technology, School of Physics and Optoelectronics, Xiangtan University, Hunan 411105, China

[c]College of Materials Science and Engineering, Taiyuan University of Technology, Taiyuan, 030024, China

[d]Hongzhiwei Technology (Shanghai) Co. Ltd., 1599 Xinjinqiao Road, Pudong, Shanghai, China
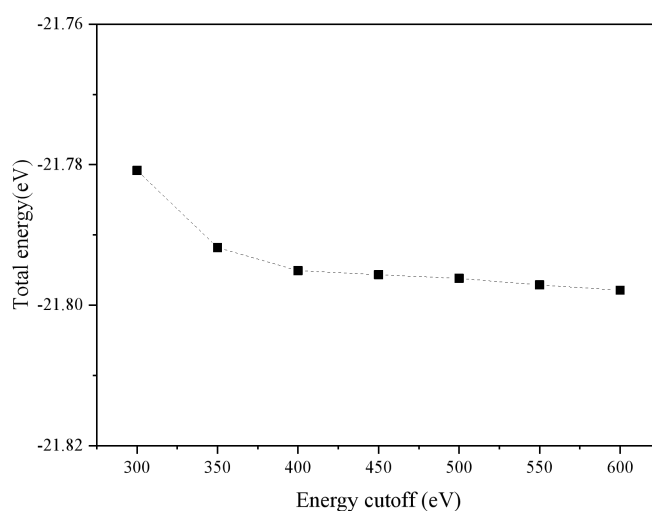
Fig. S1 The convergence for energy cutoff from 300eV to 600eV in MoS_2 monolayer unit-cell.

Table. S1 The total energy difference in scf calculation using same k-point density 3×3×1 after geometry optimization using different k-point density 1×1×1 and 3×3×1.

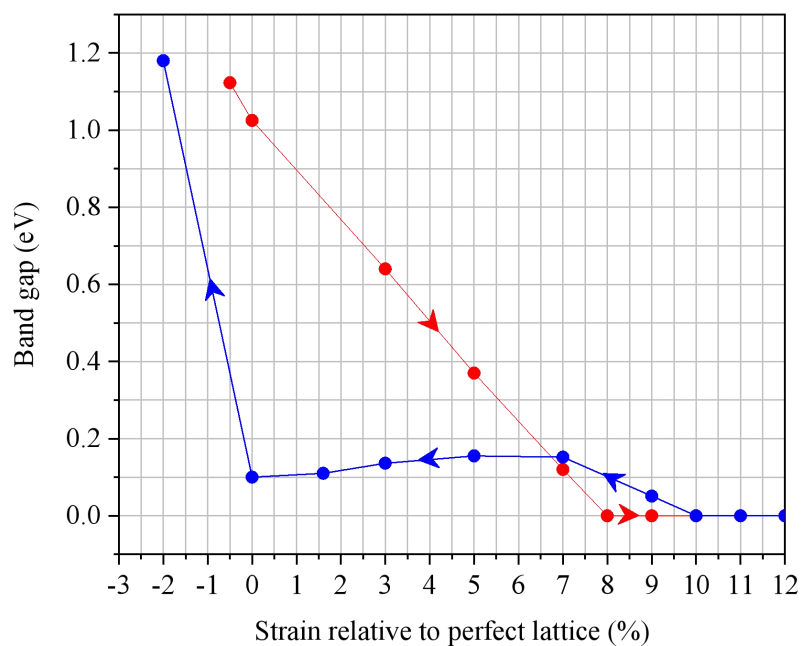| strain		tot-energy(3×3×1)	tot-energy(1×1×1)	ΔE
Load	ε=8%	-751.47259	-751.47016	0.00243
	ε=10%	-743.64421	-743.64144	0.00277
	ε=12%	-738.49087	-738.48767	0.00320
Unload	ε=1.6%	-764.23192	-764.23177	0.00015

Fig. S2 The band gap of MoS$_2$ monolayer with the DSV defect for loading (red curve) and unloading (blue curve) strains.
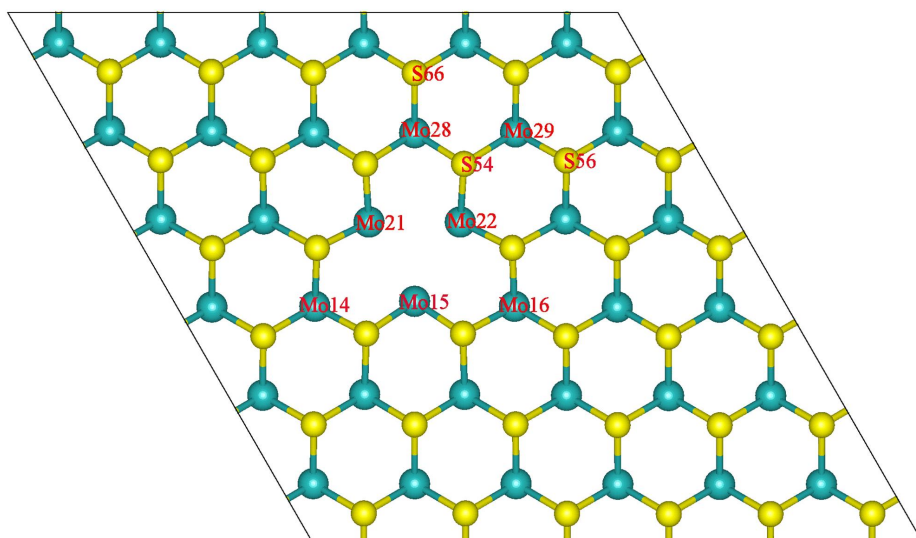

Fig. S3 Atomic indexes around the DSV defect, including the 1st-Mo atoms (Mo15, Mo21, Mo22), 2nd-Mo atoms (Mo14, Mo16, Mo28), 3rd-Mo atoms (Mo29), and the surrounding S atoms (S54, S56, S66).

Table. S2 The -ICOHP values of bonds Mo21-Mo22, S54-Mo22, S56-Mo22, Mo22-Mo29, S54-Mo28 and S66-Mo28 under different stresses.

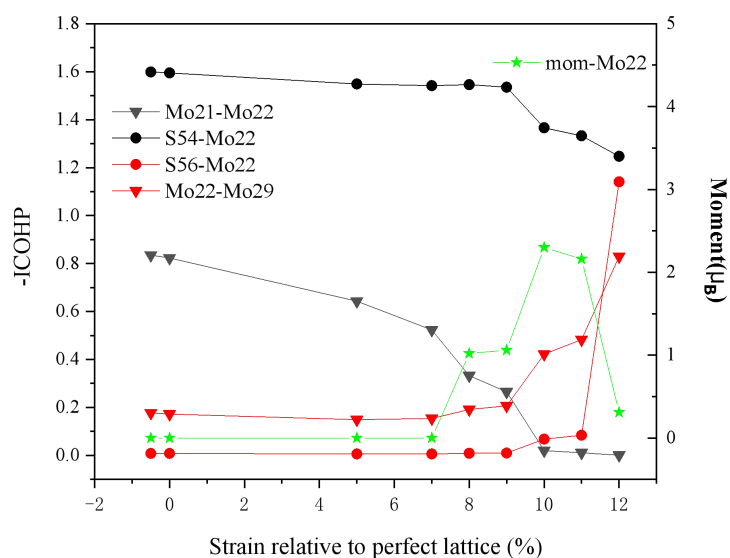|			-ICOHP					
		Spin	Mo21-Mo22	S54-Mo22	S56-Mo22	Mo22-Mo29	S54-Mo28	S66-Mo28
	perfect		0.280	1.567	0.011	0.280	1.567	1.567
Load	-0.5%		0.835	1.599	0.008	0.177	1.603	1.537
	0%		0.823	1.595	0.008	0.172	1.529	1.599
	5%		0.643	1.549	0.006	0.149	1.469	1.531
	8%	up	0.355	1.461	0.008	0.185	1.437	1.471
		dw	0.310	1.631	0.009	0.198	1.419	1.440
	9%	up	0.283	1.454	0.009	0.199	1.399	1.467
		dw	0.247	1.617	0.010	0.214	1.379	1.455
	10%	up	0.031	1.285	0.039	0.409	1.376	1.491
		dw	0.009	1.447	0.096	0.435	1.388	1.532
	11%	up	0.018	1.267	0.045	0.458	1.341	1.481
		dw	0.004	1.399	0.123	0.508	1.358	1.530
	12%	up	-0.001	1.239	1.127	0.799	1.228	1.459
		dw	0.000	1.256	1.155	0.860	1.274	1.590
Unload	10%	up	-0.001	1.310	1.058	0.883	1.325	1.476
		dw	0.000	1.308	1.073	0.914	1.365	1.581
	7%	up	-0.001	1.397	0.975	0.959	1.450	1.486
		dw	0.001	1.394	0.986	1.003	1.488	1.578
	1.6%	up	0.001	1.537	0.876	1.068	1.578	1.512
		dw	0.004	1.537	0.880	1.126	1.631	1.608

Fig. S4 The -ICOHPs (the average of up and dw) of bonds Mo21-Mo22, S54-Mo22, S56-Mo22 and Mo22-Mo29 under loading strains and the corresponding magnetic moment of Mo22 .
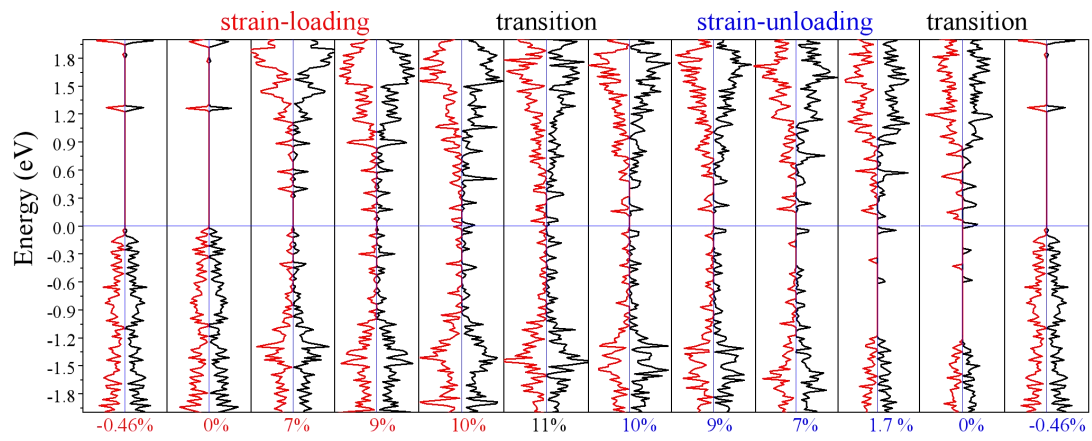
Fig. S5 The electronic density of states for the WS$_2$ monolayer with the DSV defect under different strains relative to the perfect lattice in the processes of strain loading and unloading.