

Supplementary Information for

Strain-induced dark exciton generation in rippled monolayer MoS₂

Su Yeong Lee^{a,‡}, Won Seok Yun^{b,‡}, and J. D. Lee^{a,*}

^aDepartment of Physics and Chemistry, DGIST, Daegu 42988, Republic of Korea

^bConvergence Research Institute, DGIST, Daegu 42988, Republic of Korea

*To whom correspondence should be addressed. E-mail: jdlee@dgist.ac.kr

[‡]These authors contributed equally.

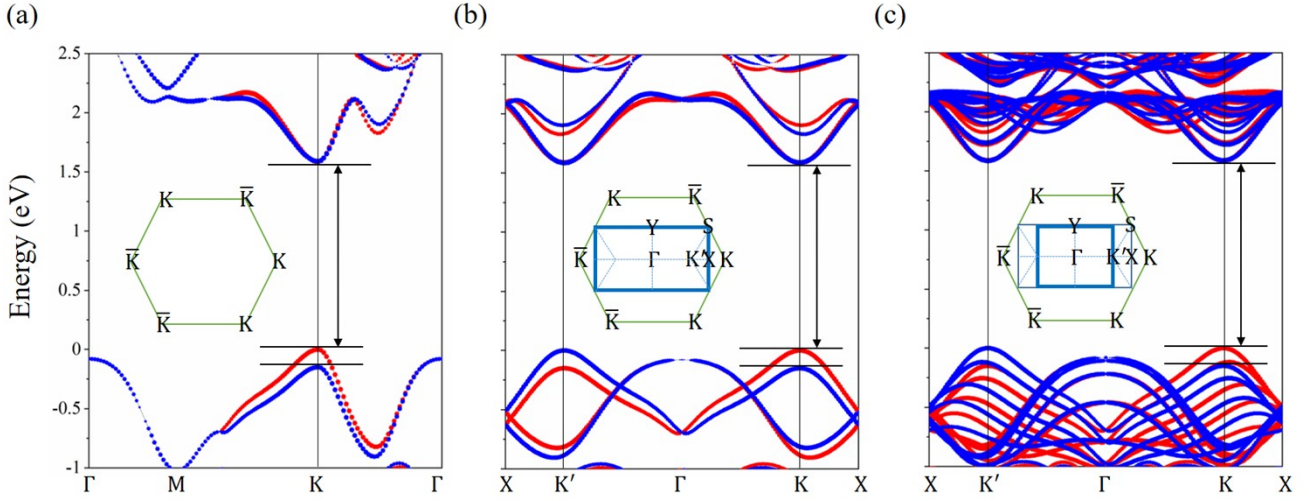


Figure S1. Electronic structure of (a) hexagonal unit cell (b) rectangular primitive cell (c) rectangular supercell with different BZs.

Figure S1 represents the electronic structure of (a) hexagonal unit cell, (b) rectangular unit cell and (c) rectangular supercell with different Brillouin zones (BZs). By properly folding a hexagonal BZ (green line) into a rectangular BZ (blue line), The BZs of our system have been created. As shown in Figs. S1(a) and S1(b), band folding occurs when the lattice changes from a hexagonal to a rectangular cell, where the high-symmetry K point of a hexagonal BZ is folded into the point situated at a $2/3$ length of the Γ -X high-symmetry path (specifically, the K' point as labeled in BZ).¹ As shown in Figs. S1(b) and S1(c), band folding occurs when a supercell is involved. In Fig. S1(b), lattice constants of a $1 \times 1 \times 1$ rectangular primitive cell are given by $a = 3.185 \text{ \AA}$ and $b = 5.516 \text{ \AA}$, and in Fig. S1(c), lattice constants of a $1 \times 8 \times 1$ rectangular supercell are given by $a = 3.185 \text{ \AA}$ and $b = 44.129 \text{ \AA}$. When the size of the supercell increases, the size of the first BZ of the corresponding supercell (SBZ) shrinks its size. As shown in the figure, the corresponding BZ shrinks from the blue rectangle line shown in Fig. S1(b) to the blue rectangle shown in Fig. S1(c). The bands in the first BZ of primitive cell fold into SBZ.²

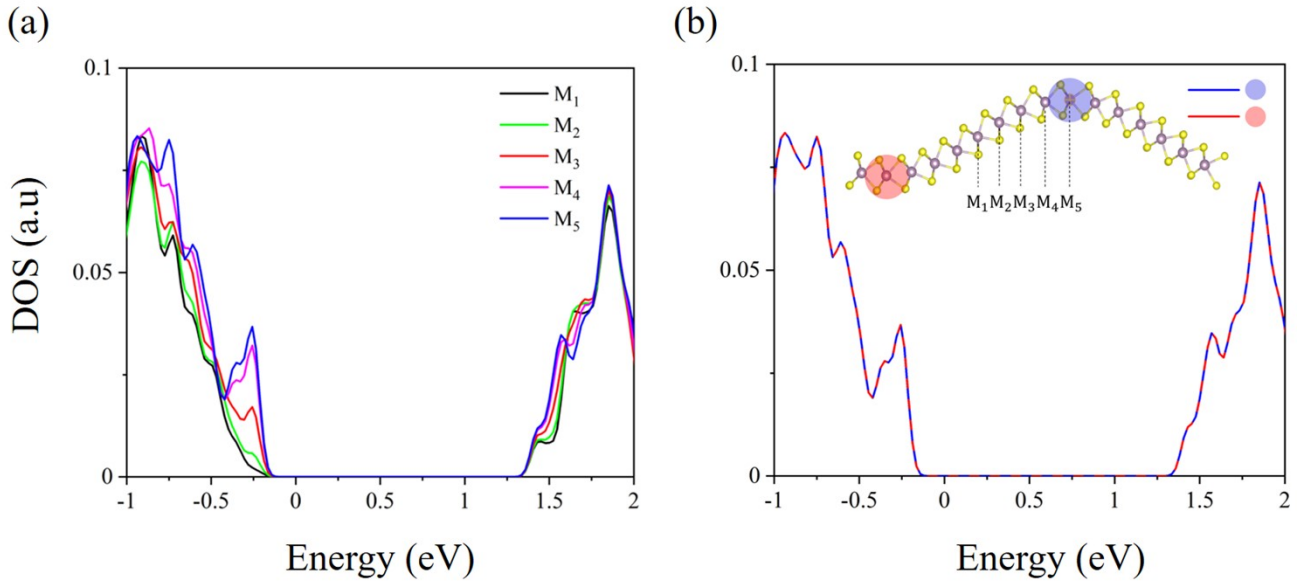


Figure S2. The atom-projected DOS of Mo atom, (a) M_i ($i=1,2,\dots,5$) and (b) valley (the circle filled with red) and chest sites (the circle filled with blue) at a particular strain of $\varepsilon \sim 9.1\%$ of rippled monolayer MoS₂

Figure S2 shows the atom-projected density of states (DOS) of a specific rippled monolayer MoS₂ at $\varepsilon \sim 9.1\%$. Compared with M_1 to M_5 in Fig. S2(a), the emergence of additional states near the VBM and CBM at a highly strained region appears distinctly. As can be seen, in highly strained regions, new states that were not seen in less strained regions appeared near the CB minimum (CBM) and the VB maximum (VBM), respectively. As shown in Fig. S2(b), DOS at the valley site completely overlap with DOS at the chest site. Note that the chest and valley are the same due to the inversion symmetry.

Table S1. Position of spin-down and spin-up bands of CBM and VBM at the K point, the CB spin-orbit splitting (Δ_{CB}^{SO}), $E_{CB\uparrow}-E_{VB\uparrow}$ and $E_{CB\downarrow}-E_{VB\downarrow}$, the direct and indirect band gaps. All energies are in eV except for Δ_{CB}^{SO} .

Strain (%)	$E_{CB\downarrow}$	$E_{CB\uparrow}$	$E_{VB\uparrow}$	$E_{VB\downarrow}$	$E_{CB\uparrow}-E_{VB\uparrow}$	$E_{CB\downarrow}-E_{VB\downarrow}$	Δ_{CB}^{SO} (meV)	E_{g_d}	E_{g_i}
0	1.4713	1.4682	-0.1178	-0.2671	1.586	1.7384	3.1	1.586	
0.45	1.5094	1.5063	-0.1053	-0.2542	1.6116	1.7636	3.1	1.6116	
1.13	1.5302	1.5273	-0.1228	-0.2709	1.6501	1.8011	2.9	1.6501	
1.36	1.5336	1.5307	-0.1316	-0.2794	1.6623	1.813	2.9	1.6623	
1.8	1.557	1.5543	-0.1318	-0.2793	1.6861	1.8363	2.7	1.6861	
2.3	1.5804	1.5777	-0.1277	-0.2752	1.7054	1.8556	2.7	1.7054	
4.5	1.584	1.5828	-0.1069	-0.2593	1.6897	1.8433	1.2	1.6897	
6.8	1.5118	1.5121	-0.1445	-0.2987	1.6566	1.8105	-0.3	1.6563	
9.1	1.4945	1.4962	-0.1285	-0.2829	1.6247	1.7774	-1.7	1.623	
11.3	1.4106	1.4134	-0.1828	-0.337	1.5962	1.7476	-2.8	1.5934	
13.6	1.3177	1.3218	-0.2423	-0.3943	1.5641	1.712	-4.1	1.56	1.4613
15.86	1.242	1.2472	-0.2893	-0.4424	1.5365	1.6844	-5.2	1.5313	1.3676
18.13	1.1476	1.1537	-0.3538	-0.5055	1.5075	1.6531	-6.1	1.5014	1.2807

References

1. N. Jena, Dimple, R. Ahammed, A. Rawat, M. K. Mohanta and A. De Sarkar, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 2016, **100**, 165413.
2. W. Ku, T. Berlijn and C.C. Lee. *Phys. Rev. Lett.*, 2010, **104**, 21640