

Supplementary Data

Dipole Moment and Pressure Dependent Interlayer Excitons in MoSSe/WSSe Heterostructures

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1. The atomic orbital distributions of the three stacking configurations at the top of the valence band and the bottom of the conduction band at K point.

Table S1 The detailed atomic orbital distribution of the three stacking configurations of VBM and CBM at the K-point.

	VBM	CBM
1-SSe	65.2%Mo($d_{xy}+d_{x^2-y^2}+d_{xz}+d_{yz}$) +7.1%Se ^{Mo} (p_x+p_y) +5%S ^{Mo} (p_x+p_y) +0.2%Mo(p_x+p_y) +0.2%W($d_{xy}+d_{yz}+d_{xz}+d_{x^2-y^2}$) +1%S ^W (p_z)+1% S ^W (s)	65.3%W(d_z^2)+6%W(s) +2.4%W($d_{yz}+d_{xz}$) +0.2%Mo(d_z^2)+2%S ^W (p_x+p_y) +2.4%Se ^W (p_x+p_y) +0.5%Se ^W ($d_{xy}+d_{yz}+d_{xz}+d_{x^2-y^2}$)
2-SeSe	56%W($d_{xy}+d_{x^2-y^2}+d_{yz}+d_{xz}+p_x+p_y$) +5.6%S ^W (p_x+p_y) +8.3%Se ^W ($p_y+p_x+d_{yz}+d_{xz}$) +0.1%Mo(d_z^2)	74.5%Mo(d_z^2)+3.9%Mo(s) +0.1%W(d_z^2) +2.9%S ^{Mo} (p_x+p_y) +3.4%Se ^{Mo} ($p_x+p_y+d_{xy}+d_{x^2-y^2}$)
3-SS	56.2%W($d_{xy}+d_{x^2-y^2}+d_{yz}+d_{xz}+p_x+p_y$) +5.7%S ^W (p_x+p_y) +8.3%Se ^W ($p_y+p_x+d_{yz}+d_{xz}$)	74.7%Mo(d_z^2)+3.9%Mo(s) +2.9%S ^{Mo} (p_x+p_y) +3.5%Se ^{Mo} ($p_x+p_y+d_{xy}+d_{x^2-y^2}$)

Table S2 Dipole moments (unit:Debye) of three stacking configurations (including 2H phase and 1T phase).

	1-SSe	2-SeSe	3-SS	1-SSe(1T)	2-SeSe(1T)	3-SS(1T)
Dipole moment	0.347	0.023	0.017	0.211	0.040	0.037

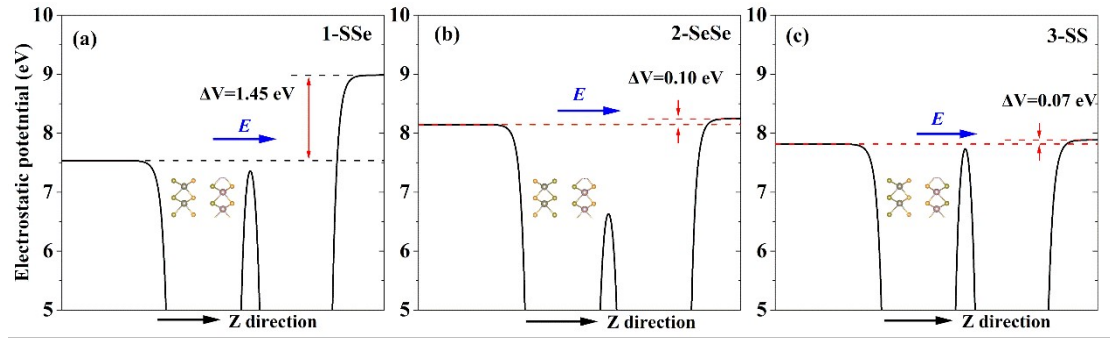


Fig. S1 The macroscopic average electrostatic potential of (a) 1-SSe, (b) 2-SeSe and (c) 3-SS.

2. The band structures of 1-SSe with G_0W_0 results at 0 GPa, 2 GPa and 4 GPa, respectively. The direct band gap and the indirect band gap are indicated as the pressure increases. The dashed line is the energy valley marked for convenience.

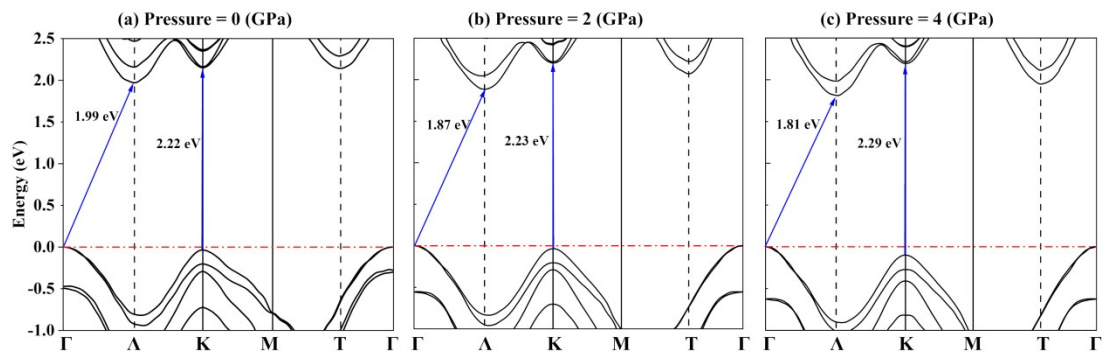


Fig. S2 The band structures of 1-SSe at (a) 0 GPa, (b) 2 GPa and (c) 4 GPa, respectively.

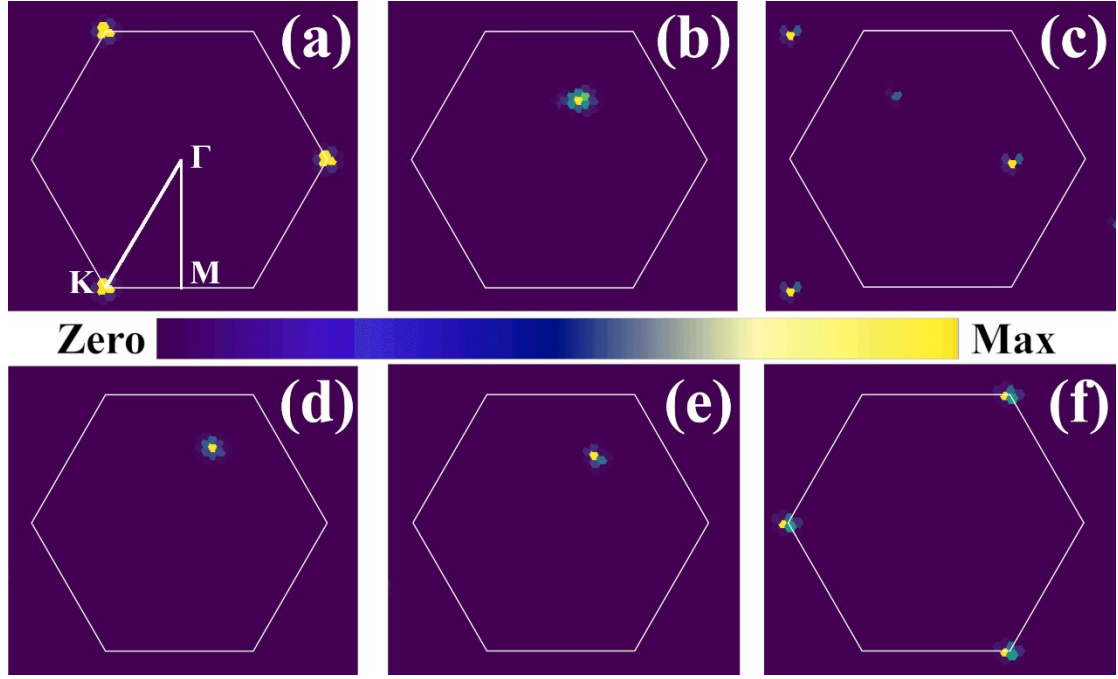


Fig. S3 The excitonic weights of IX_0 without pressure under different momentum in the first Brillouin zone. (a) K-K valley. (b) Γ -T valley. (c) K- Λ valley. (d) K-T valley. (e) Γ - Λ valley. (f) Γ -K valley.