Electronic Supplementary Information (ESI)

Interfacial hybridization of Janus MoSSe and BX (X= P, As) monolayers for ultrathin excitonic solar cell, nanopiezotronics and low-power memory devices

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Formalism:

Mechanical constants: 2D layer modulus: $\gamma^{2D} = \frac{1}{2}[C_{11} + C_{12}]$ (1)

Young's modulus $(\Upsilon) = \frac{C_{11}^2 - C_{12}^2}{C_{11}}$ (2)

Poisson ratio $(\nu) = C_{12}/C_{11}$ (3)

Shear modulus $(G) = C_{66}$ (4)

Intrinsic strength $\sigma_{int} \sim \frac{\Upsilon}{9}$ (5)

Bending modulus $D = \frac{\Upsilon h^2}{12(1-\nu^2)}$ (6), where h is the thickness of the nanosheet (~ 7.35Å)

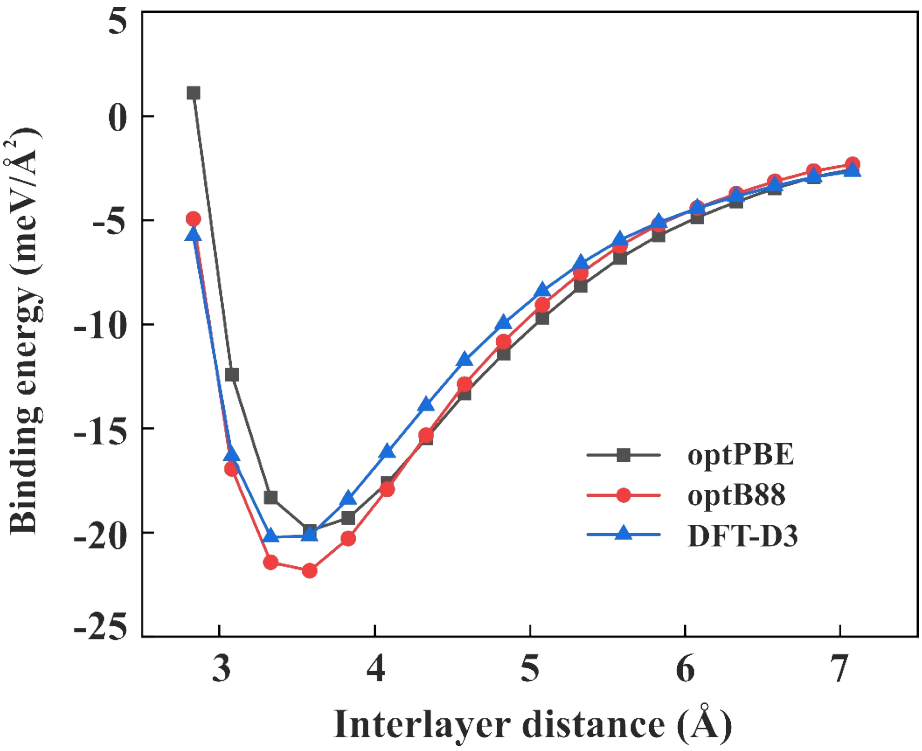

Figure S1. Interlayer distance vs binding energy curve of BP/MoSSe using different van der Waals correction

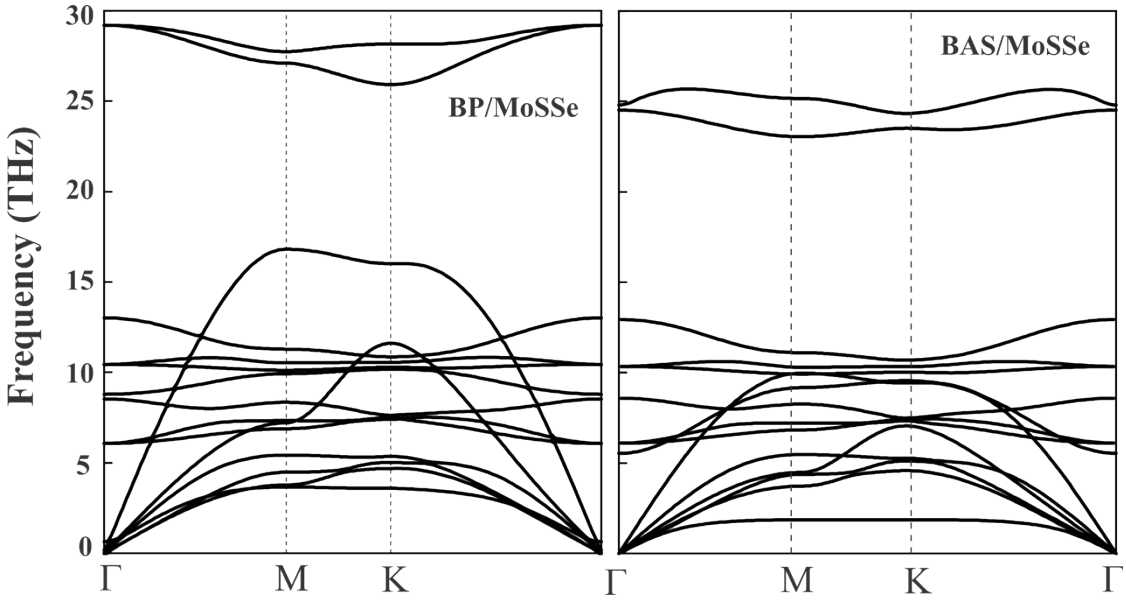

Figure S2. Phonon dispersion curve of BX/MoSSe vdWHs.

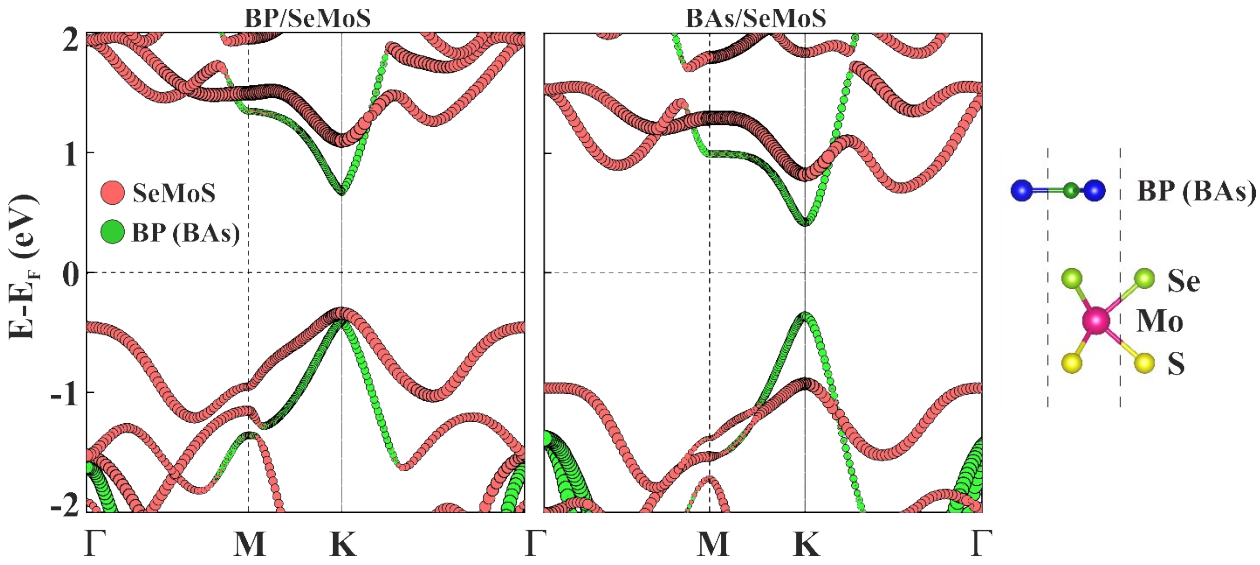

Figure S3. Electronic band structure of BP(BAs)/SeMoS heterostructure calculated using GGA-PBE

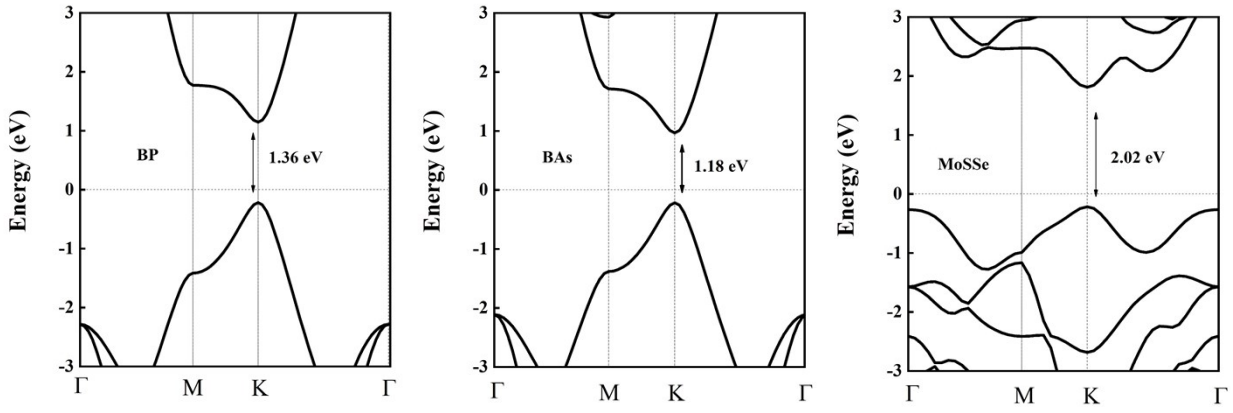

Figure S4. The electronic band structure of individual monolayers calculated using HSE06.

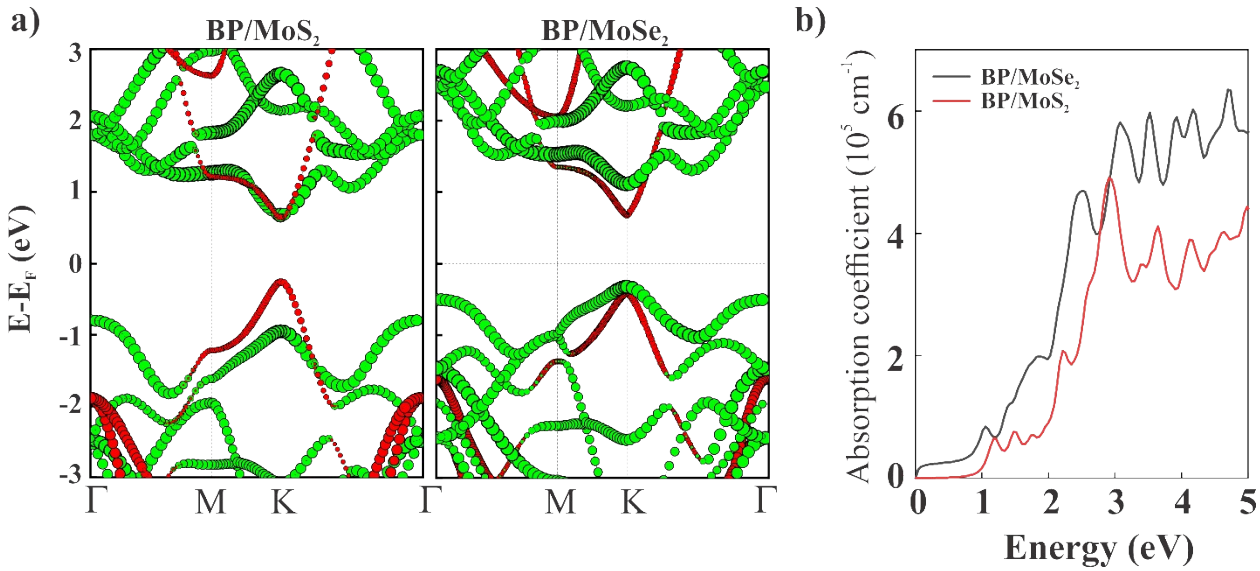

Figure S5. Electronic band structure of BP/MoS_2 and $BP/MoSe_2$ vdWH and their absorption coefficient

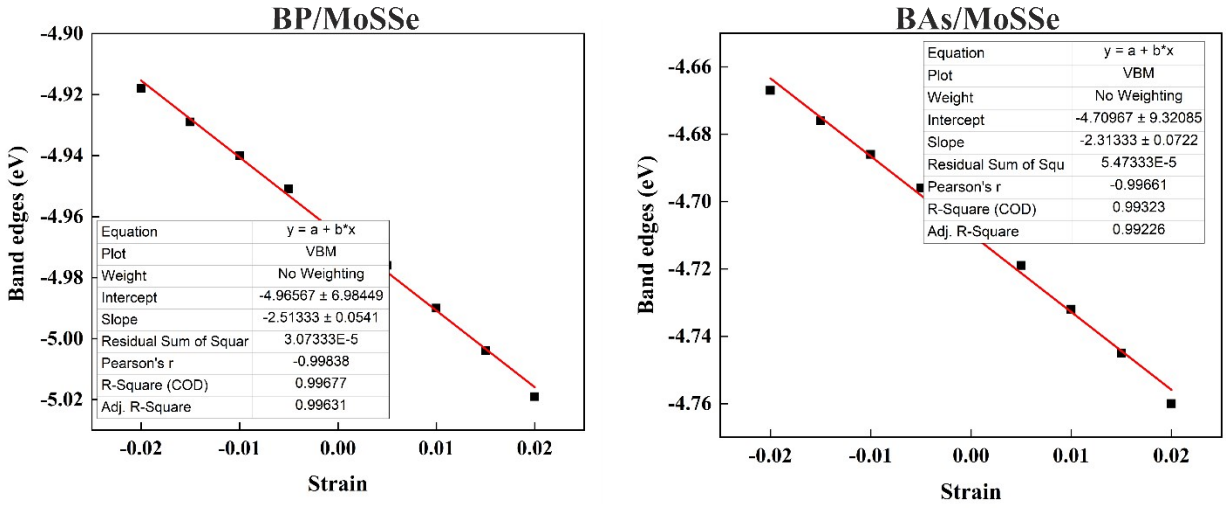

Figure S6. Deformation potential of holes calculated for BX/MoSSe vdWH

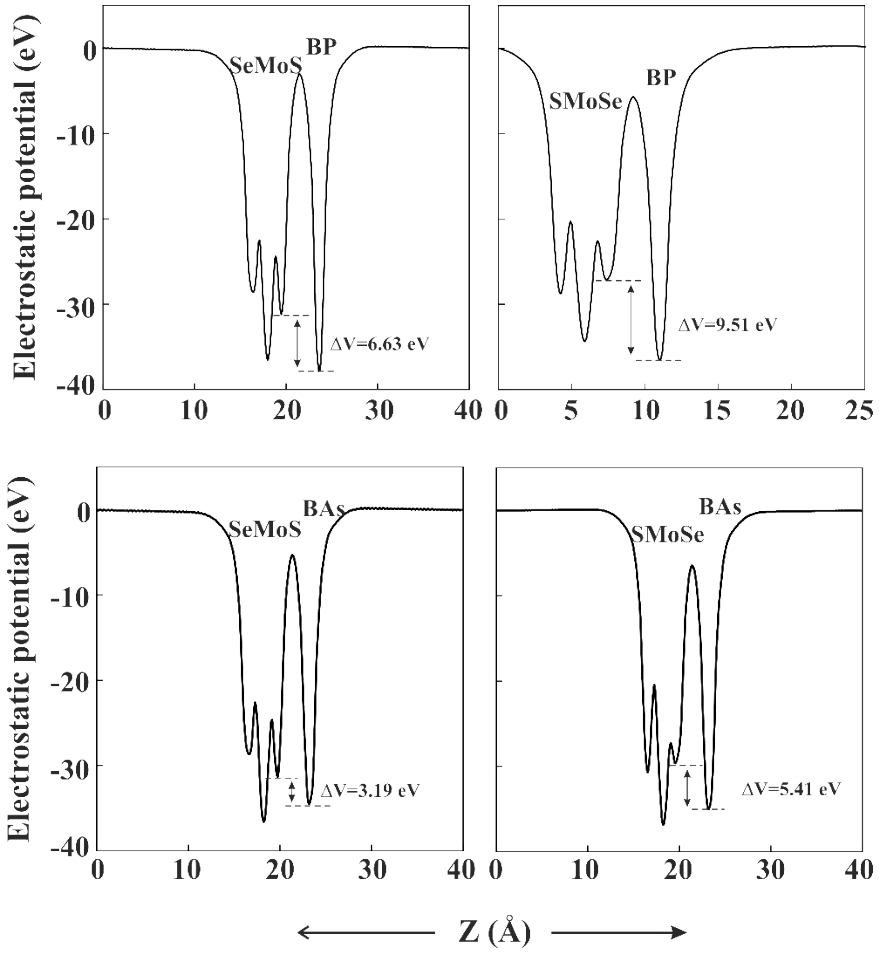

Figure S7. Electrostatic potential energy profile of different vdWHs.

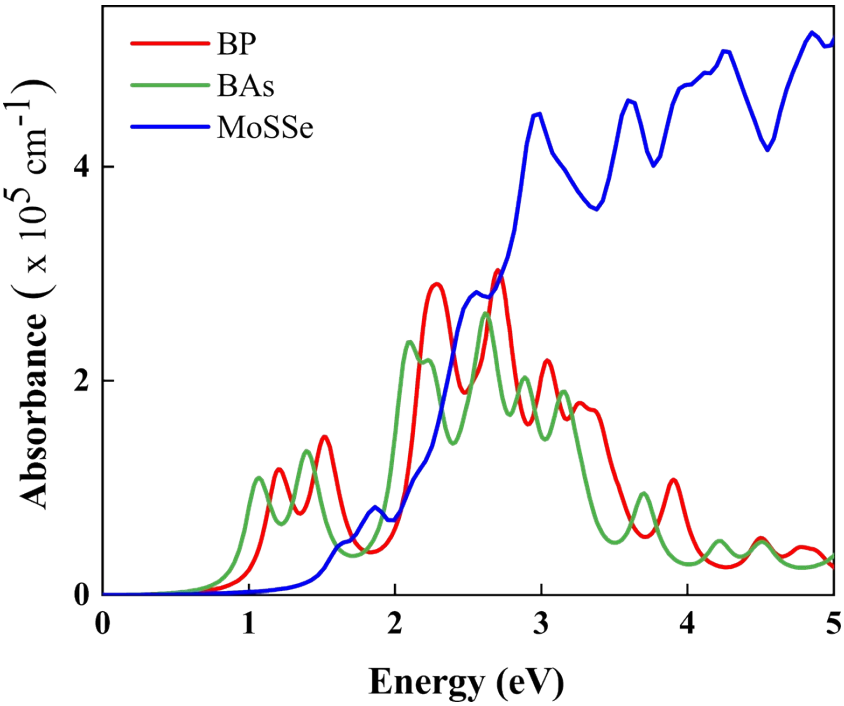

Figure S8. The optical absorption spectra of monolayers.

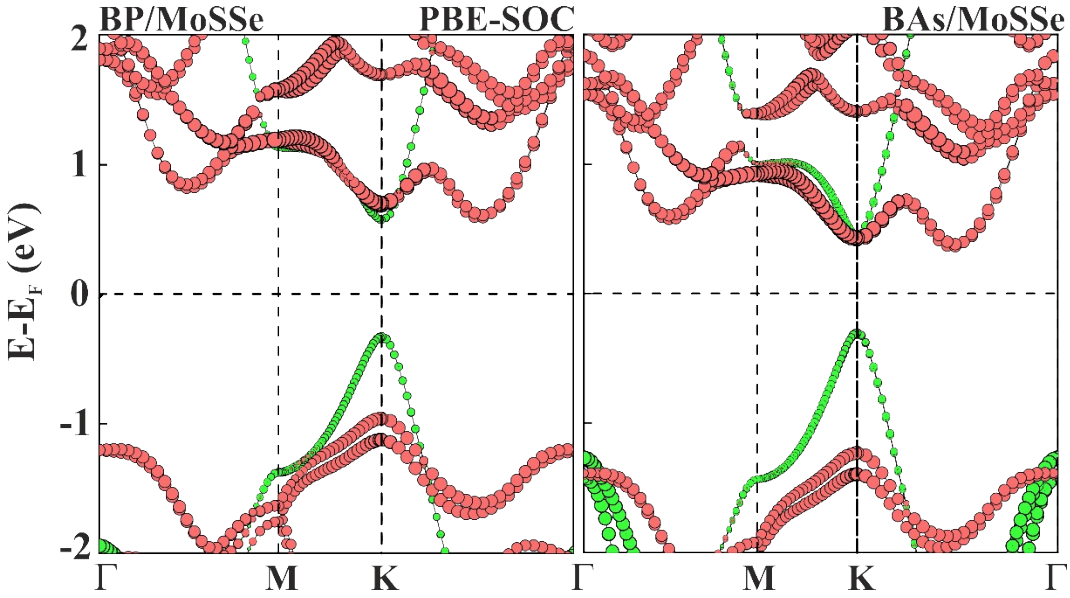

Figure S9. The electronic band structure of BX/MoSSe including SOC

Table-S1 Calculated relaxed ion (Electronic + Ionic) piezoelectric tensor e_{ij} (unit: C/m²) and total elastic modulus C_{ij} (unit: GPa) of BP/MoSSe and BAs/MoSSe heterobilayer							
e_{ij}				C_{ij}			
BP/MoSSe							
	1	**2**	**3**		**1**	**2**	**3**
1	-0.00134	-0.00108	0.00012	**1**	70.67	17.95	0.21
2	0.0349	-0.03354	-0.0001	**2**	17.95	69.8	-0.29
3	-0.01104	-0.01104	-0.01583	**3**	0.216	-0.293	1.06
BAs/MoSSe							
	1	**2**	**3**		**1**	**2**	**3**
1	0.00738	0.00053	0.00096	**1**	66.245	15.60	-0.088
2	0.04618	-0.05079	-0.0006	**2**	15.60	66.36	-0.152
3	-0.00021	-0.00022	-0.01086	**3**	-0.0885	-0.152	1.423

Note that the total elastic modulus C_{ij} is calculated with a high dense k-mesh of 16×16×1 and higher energy cut-off of 700 eV, as suggested by VASP. The piezoelectric coefficients (d_{21}) of BP, BAs have been calculated[1] to be 1.81 pm/V and 2.3 pm/V respectively which are in excellent agreement with other reports.[2]

References:

1 M. K. Mohanta, Dimple, A. Rawat, N. Jena, R. Ahammed and A. D. Sarkar, *Physica E: Low-dimensional Systems and Nanostructures*, 2020, **124**, 114222.

2 J. Shi, C. Han, X. Wang and S. Yun, *Physica B: Condensed Matter*, 2019, **574**, 311634.