Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Theoretical Perspective of the Enhanced Photocatalytic Properties by Forming Tetragonal ZnS/ZnSe Hetero-Bilayer

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Typical INCARs for geometry optimization, as well as GW and BSE calculations:

Geometry Optimization:	GW:	BSE:
ALGO = Fast	LWAVE = . TRUE.	LWAVE = . TRUE.
NSIM = 4	ALGO = GW0	ALGO = BSE
LREAL = .FALSE.	NOMEGA = 96	LBSE = .TRUE.
NELM = 400	LREAL = .FALSE.	NOMEGA = 96
NSW = 400	NELM = 1	LREAL = .FALSE.
ISIF = 3	NSW = 0	NELM = 1
IBRION = 2	ENCUT = 500.0	NSW = 0
ENCUT = 500.0	ENCUTGW= 150.0	ENCUT = 500.0
PREC = Accurate	PREC = Accurate	ENCUTGW= 150.0
EDIFF = 1E-5	EDIFF = 1E-5	PREC = Accurate
EDIFFG = -0.01	ISMEAR = -5	EDIFF = 1E-5
ISMEAR = -5	NBANDS = 192	ISMEAR = -5
IVDW=12	PRECFOCK=F	NBANDS = 192
		NBANDSO= 32
		NBANDSV= 30
		PRECFOCK=F

POSCAR for t-ZnS/ZnSe BL:

t-ZnS/ZnSe BL
1.00000000000000
4.0086111083712943 0.0000000000000000 0.0000000000000000
0.0000000000000000 4.0086111083712943 0.0000000000000000
0.0000000000000000 0.0000000000000000 28.9515883000000009
Zn Se S
4 2 2
Direct
0.0000000000000000 0.0000000000000000 0.4118548059427786
0.5000000000000000 0.5000000000000000 0.4118548059427786
0.5000000000000000 0.5000000000000000 0.5881512416197066
0.0000000000000000 0.0000000000000000 0.5881512416197066
0.5000000000000000 0.0000000000000000 0.4640977029137209
0.0000000000000000 0.5000000000000000 0.3591442952752337
0.5000000000000000 0.0000000000000000 0.6341382376822048
0.0000000000000000 0.5000000000000000 0.5426076690038701

Pseudopotentials (version potpaw_PBE.54):

Standard PAW potentials were employed for geometry optimization, with valence configurations of $3d^{10}4s^2$ for Zn, $3s^23p^4$ for S, and $4s^24p^4$ for Se.

PAW potentials designed for GW calculation were employed for GW calculation, with valence configurations of $3d^{10}4s^2$ for Zn, $3s^23p^4$ for S, and $4s^24p^4$ for Se.

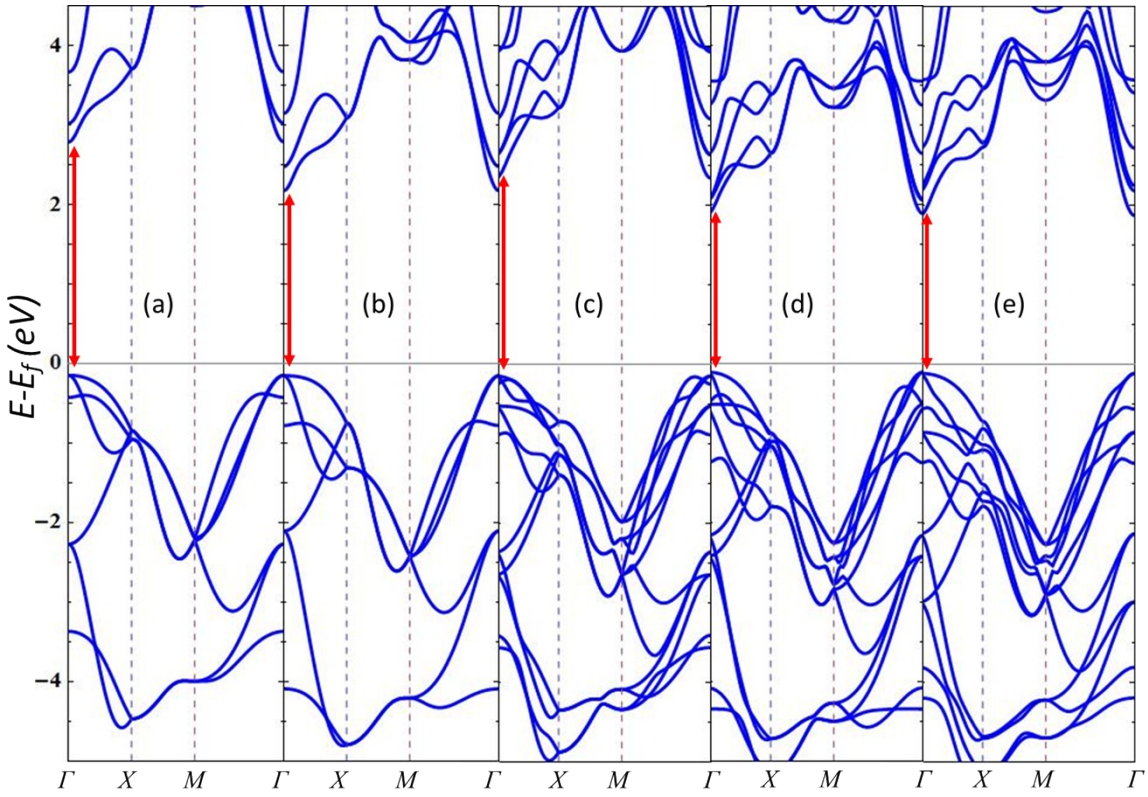

Figure S1. Band Structures of t-ZnS SL (a), t-ZnSe SL (b), t-ZnS BL (c), t-ZnSe BL (d), and t-ZnS/ZnSe BL (e), calculated by the PBE-D3.