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

Carrier mobility and Optical properties of a type-II GaSe/ZnS heterostructure as photocatalyst: A First-Principles Study

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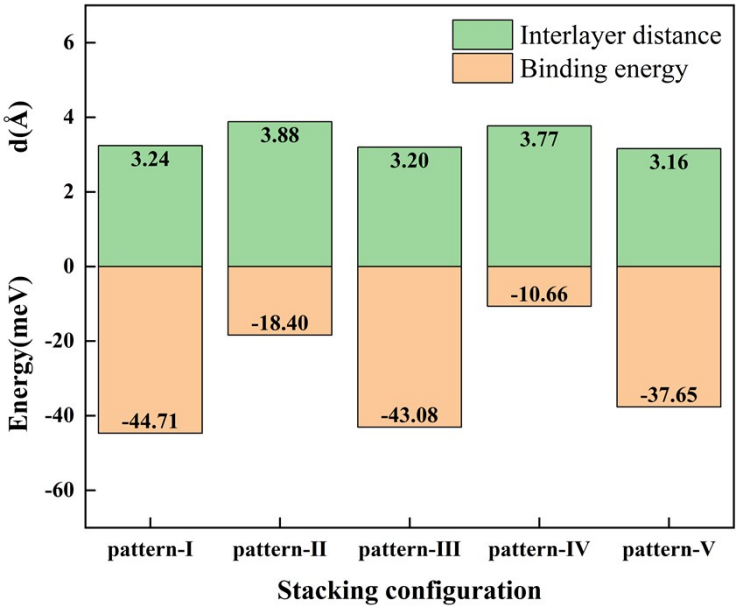

Fig.S1 Binding energy E_b (eV) and layer spacing d (Å) for five different conformations.

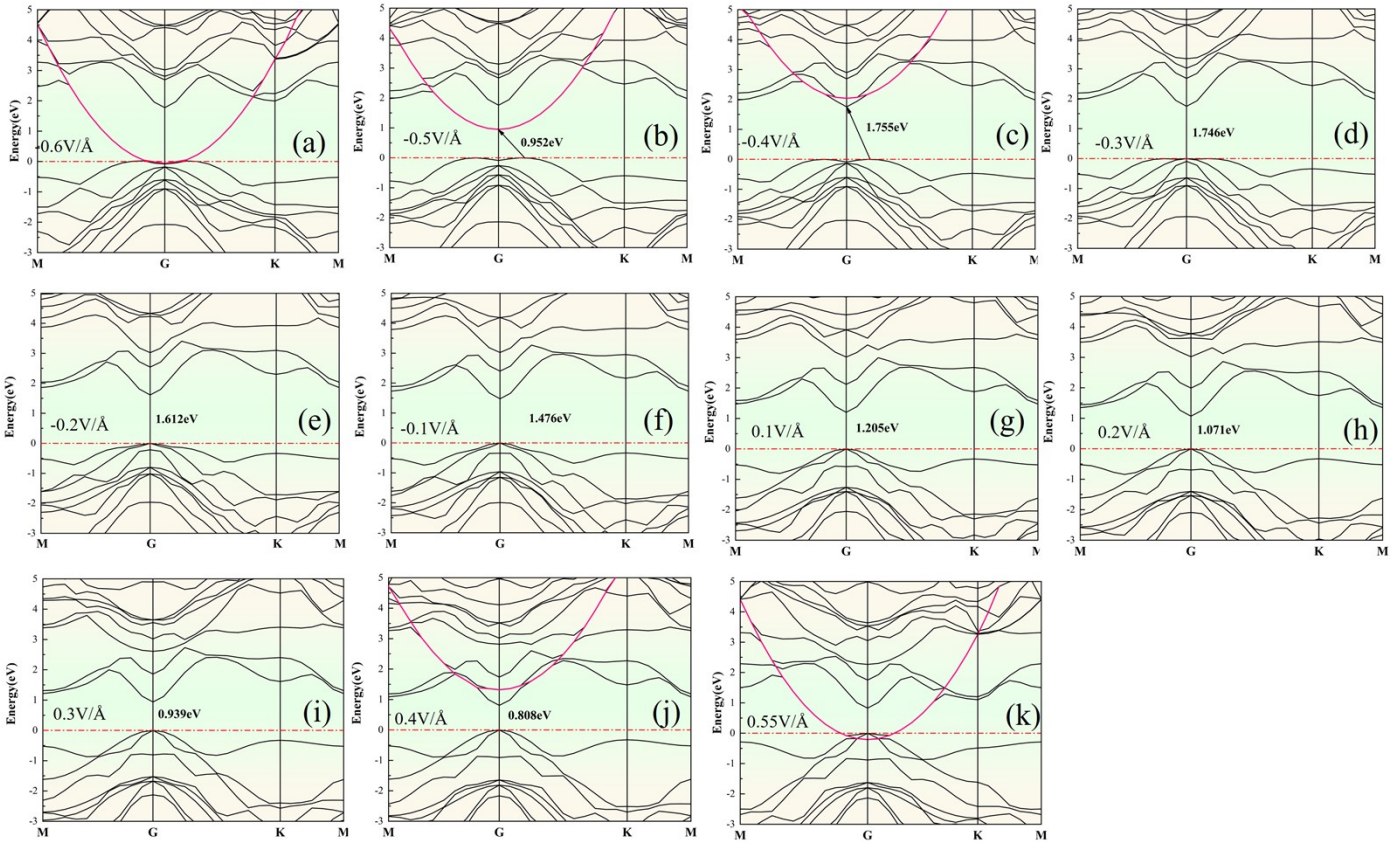

Fig.S2 (a-k) Electronic band structures of GaSe/ZnS vdWH under different electric fields (-0.6 V/Å to +0.55 V/Å).

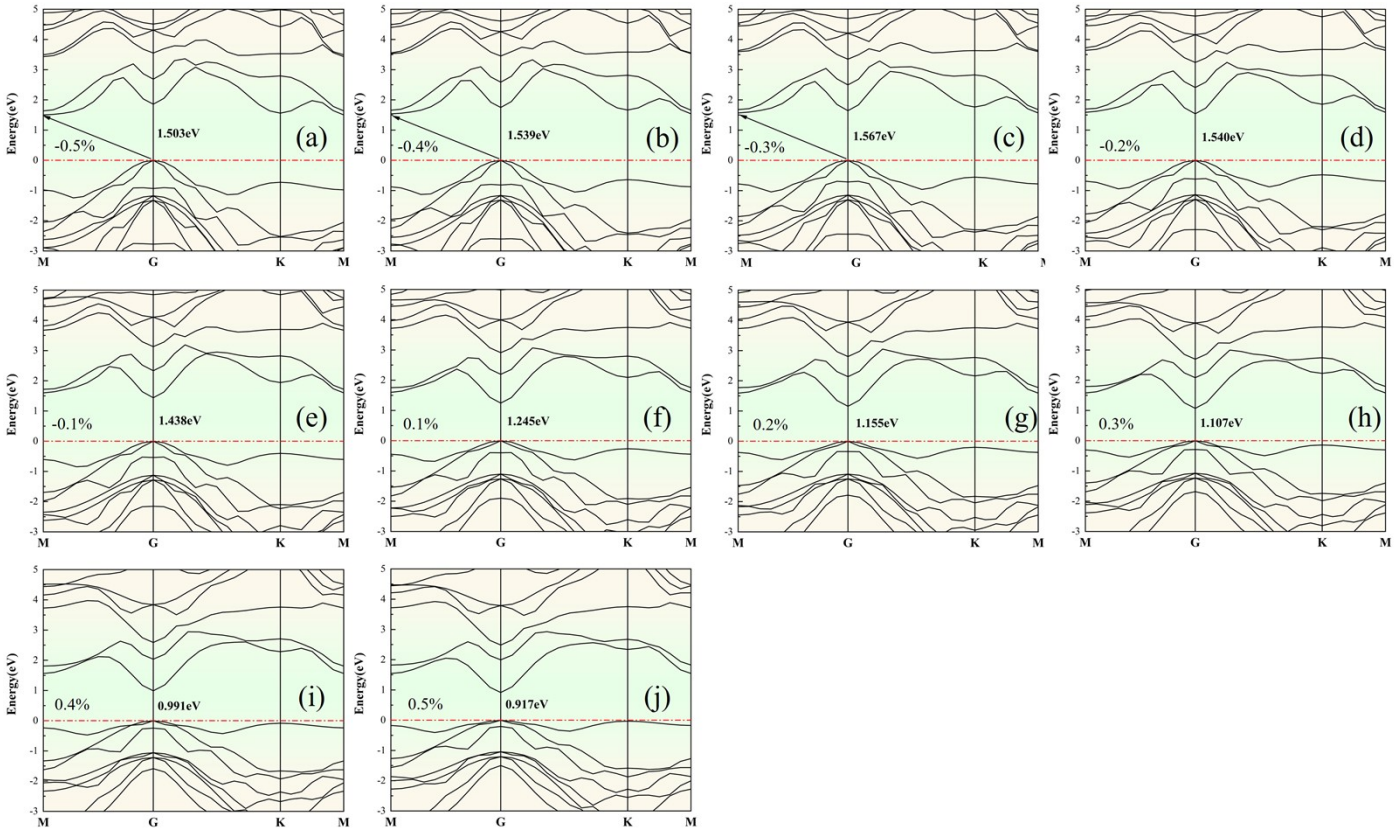

Fig.S3 (a-j) Electronic band structures of GaSe/ZnS vdWH under different biaxial strain (-5% to -5%).

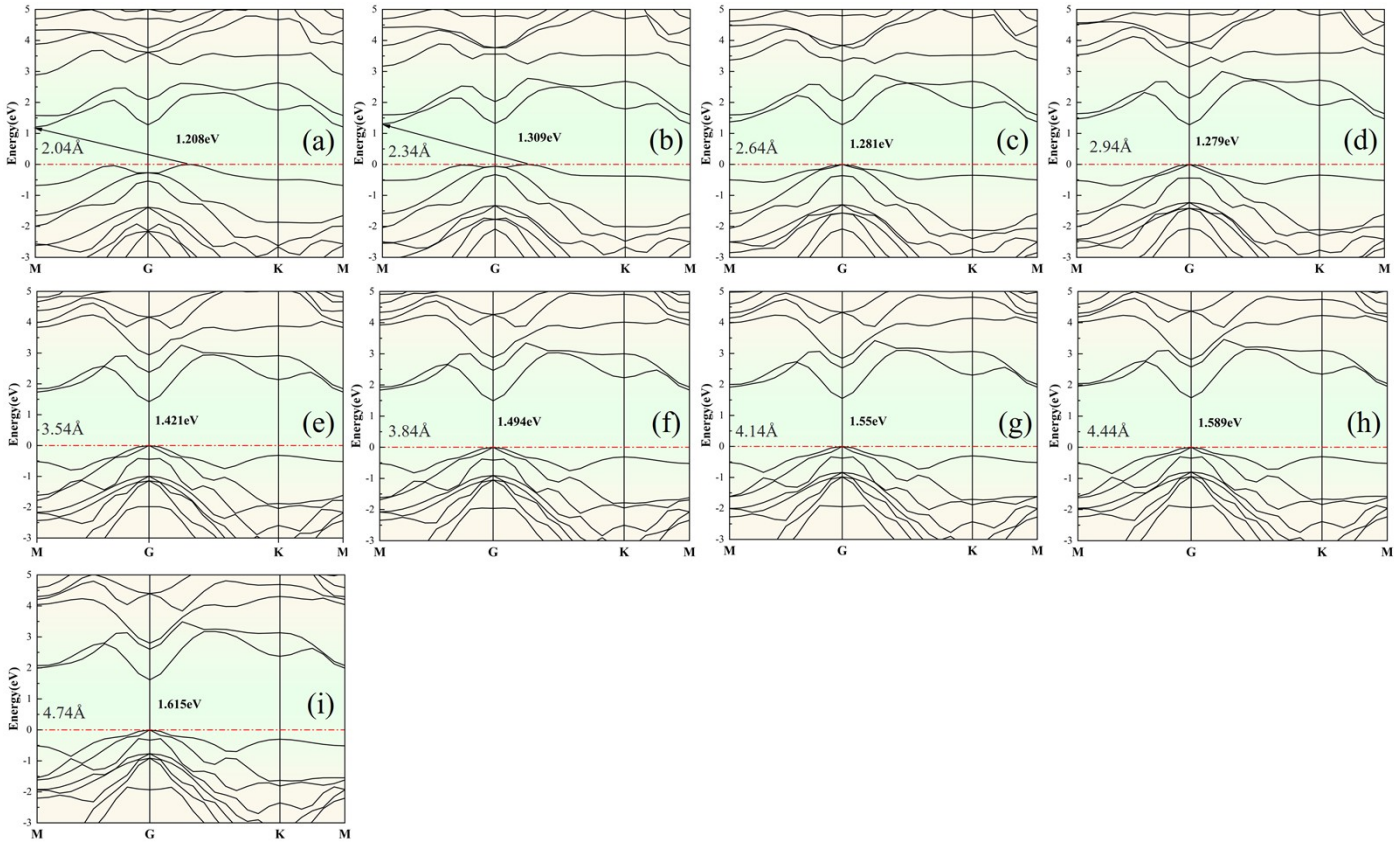

Fig.S4 (a-i) The band structure of GaSe/ZnS vdWH with interlayer spacing ranging from 2.04 Å to 4.74 Å.

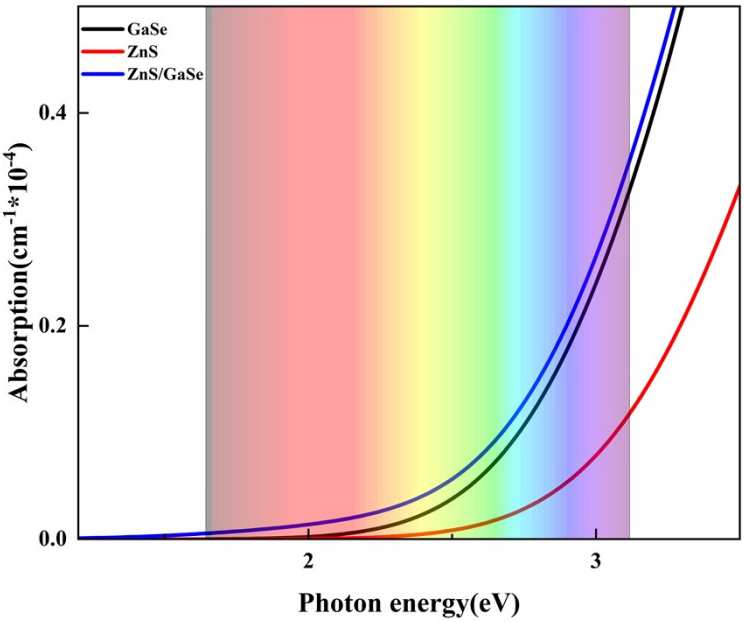

Fig.S5 The Inset of Fig. 11 (a)