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Electronic Supplementary Information

Type-II GaSe/GeS heterobilayer with strain enhanced photovoltaic properties and external electric field effects

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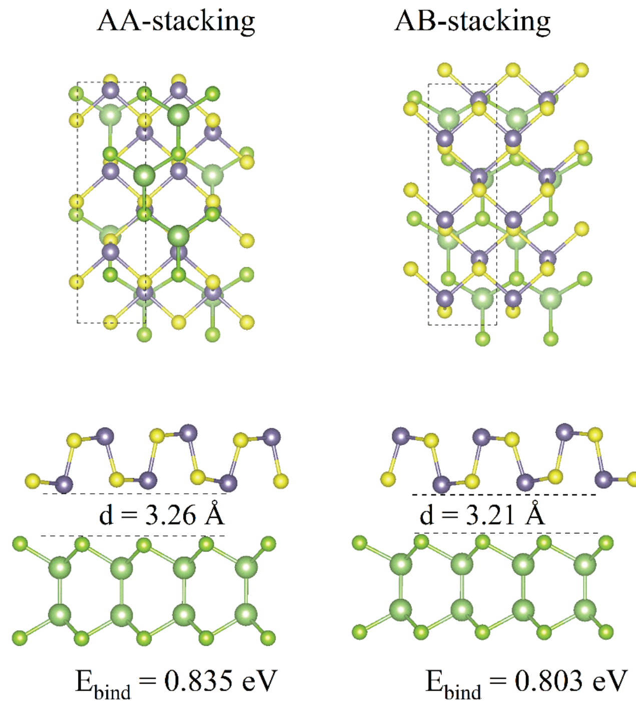

Fig. S1. Top and side views of GaSe/GeS heterobilayers for AA and AB stacking configuations.

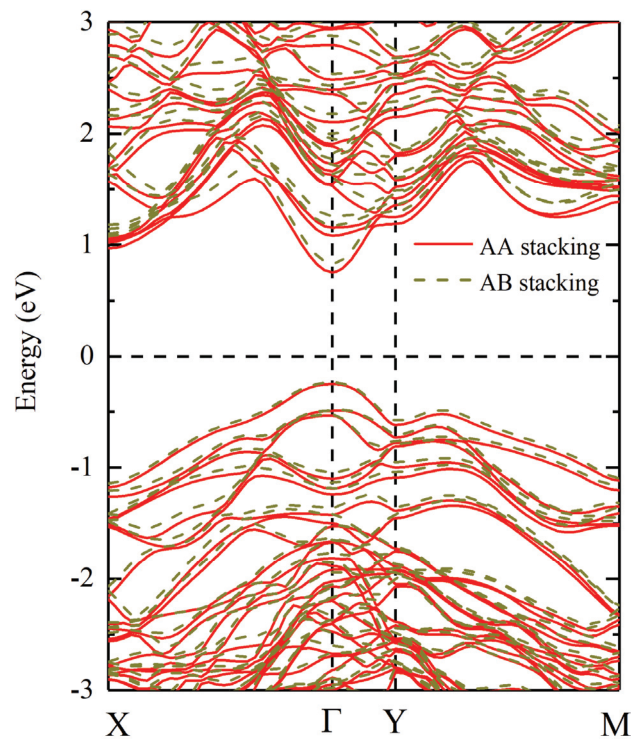

Fig. S2. The comparation of band structures of GaSe/GeS heterostructures stacked in AA, AB sequences, calculated by using PBE with DFT-D2.

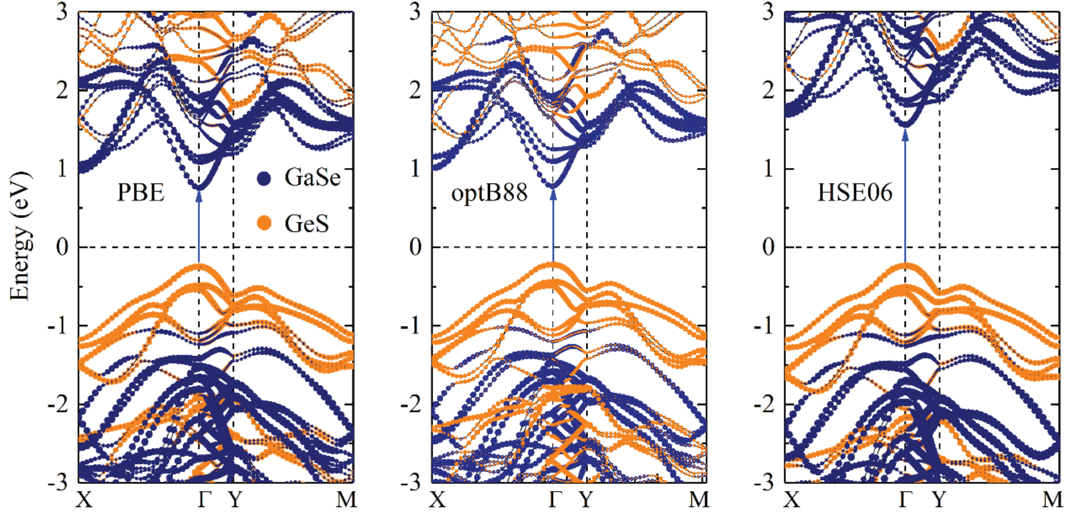

Fig. S3. Projected band structure of GaSe/GeS heterobilayer calculated by using PBE with DFT-D2, PBE with optB88, HSE06 with DFT-D2 method.

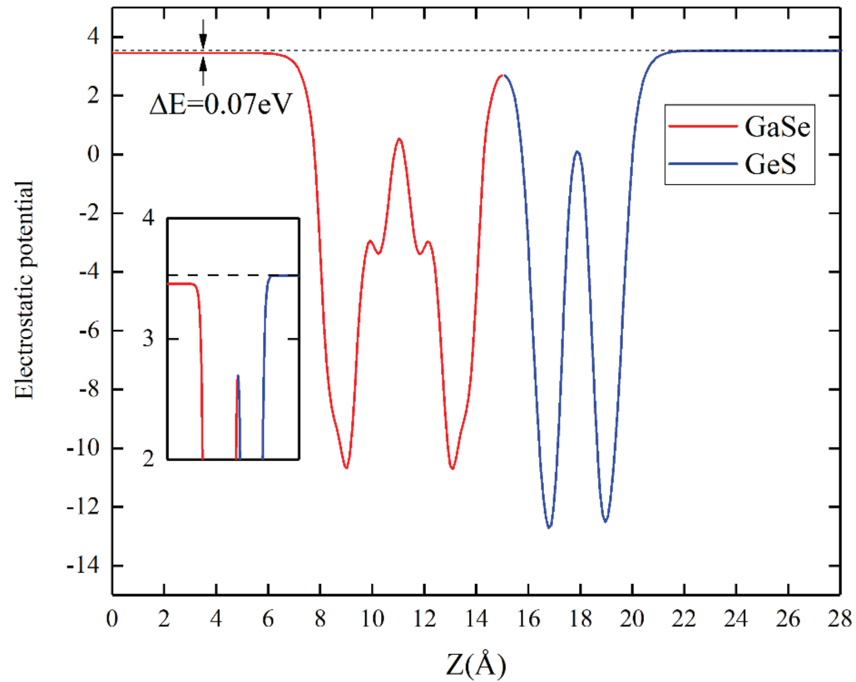

Fig. S4. Plane averaged electronic potential along the perpendicular direction of the GaSe/GeS heterostructors. The inset represents the enlarged electrostatic potential step.

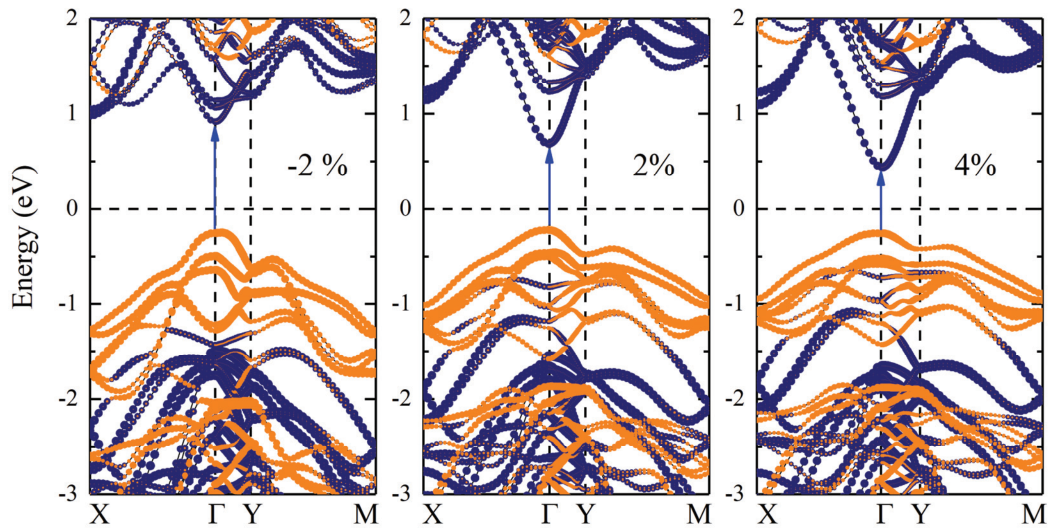

Fig. S5. Projected band structures with biaxial strain of -2%, 2%, 4% for GaSe/GeS heterostructure.

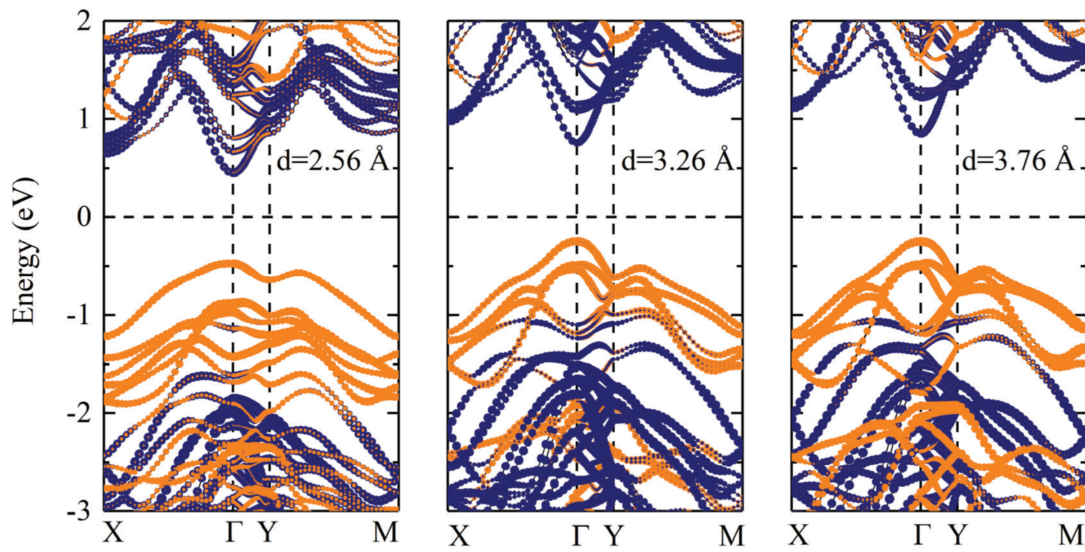

Fig. S6. Projected band structures with interlayer distances of 2.56 Å, 3.26 Å, 3.76 Å for GaSe/GeS heterostructure.