

**Supplementary Information For**  
**Intrinsic type-II van der waals heterostructures based on graphdiyne**  
**and XSe (X=Mo, W): a first-principles study**

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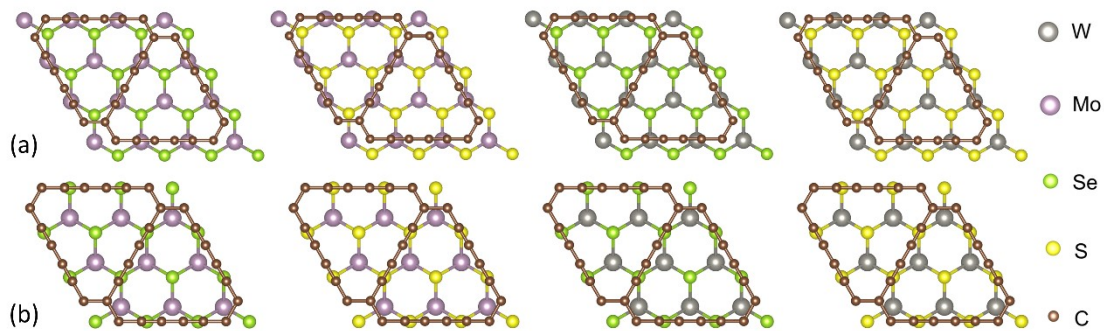


Figure S1. Top view of two stacking configurations of G@SeMoS, G@SMoSe, G@SeWS, and G@SWSe heterostructures, respectively. (a) pattern-ii (b) pattern-iii

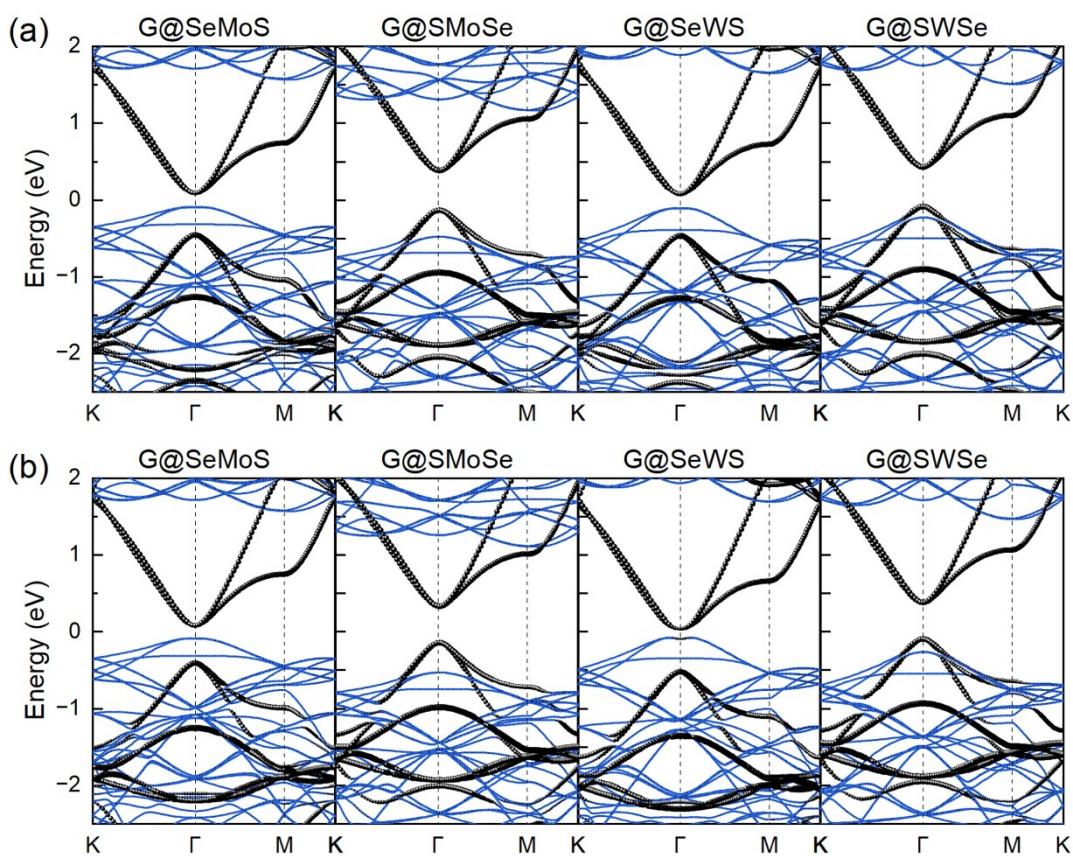


Figure S2. (a) Band structures of pattern-ii G@SeMoS, G@SMoSe, G@SeWS, and G@SWSe heterostructures, respectively. (b) Band structures of pattern-iii G@SeMoS, G@SMoSe, G@SeWS, and G@SWSe heterostructures, respectively. The black dots and blue lines in the band structures represent the projected band of GDY and XSSe (X=Mo,W), respectively.