Supplemental Information

Design and regulation of high-performance photovoltaic systems based on two-dimensional novel KAgSe/KAgX (X = S, Te) van der Waals heterojunctions

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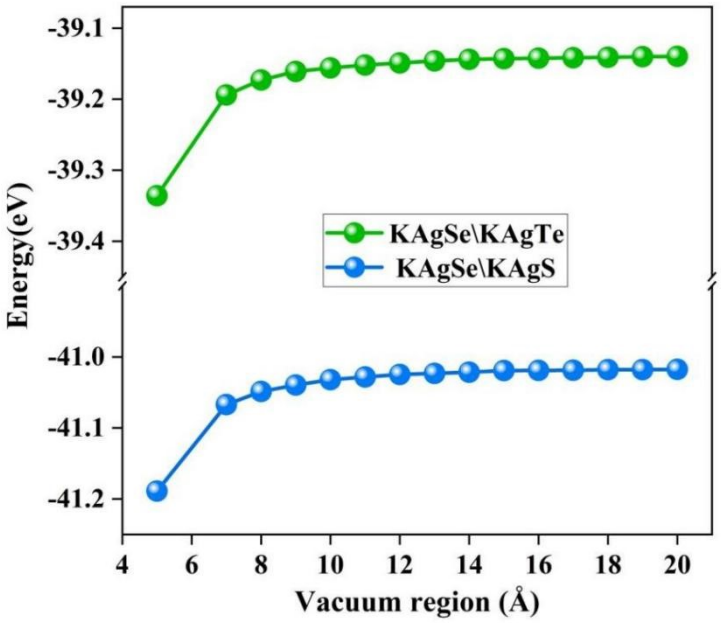

Fig. S1 The total energy as a function of the vacuum region for KAgSe/KAgX (X = S, Te) vdWHs.

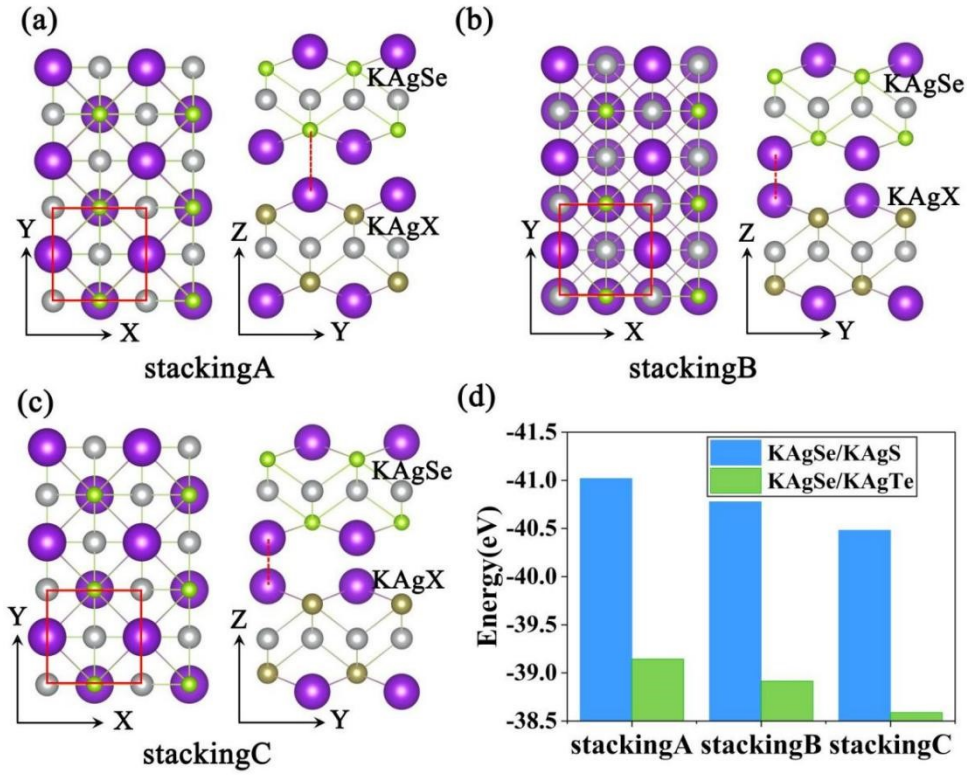

Fig. S2 (a-c) Different stacking modes for the KAgSe/KAgX (X = S, Te) vdWHs. (d) Total energy under the different stacking modes for KAgSe/KAgX (X = S, Te) vdWHs.

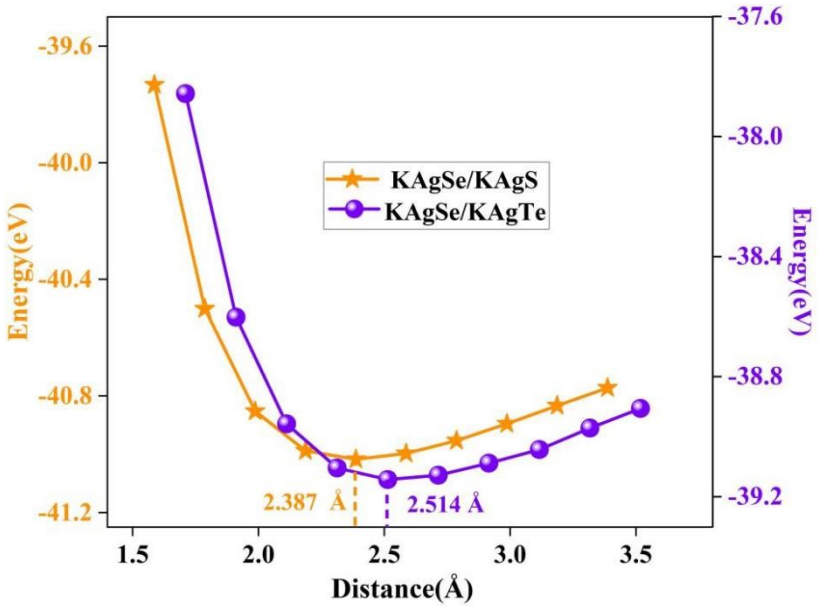

Fig. S3 Variation in the total energies, with interlayer distance d (Å) in KAgSe/KAgX (X = S, Te) vdWHs.

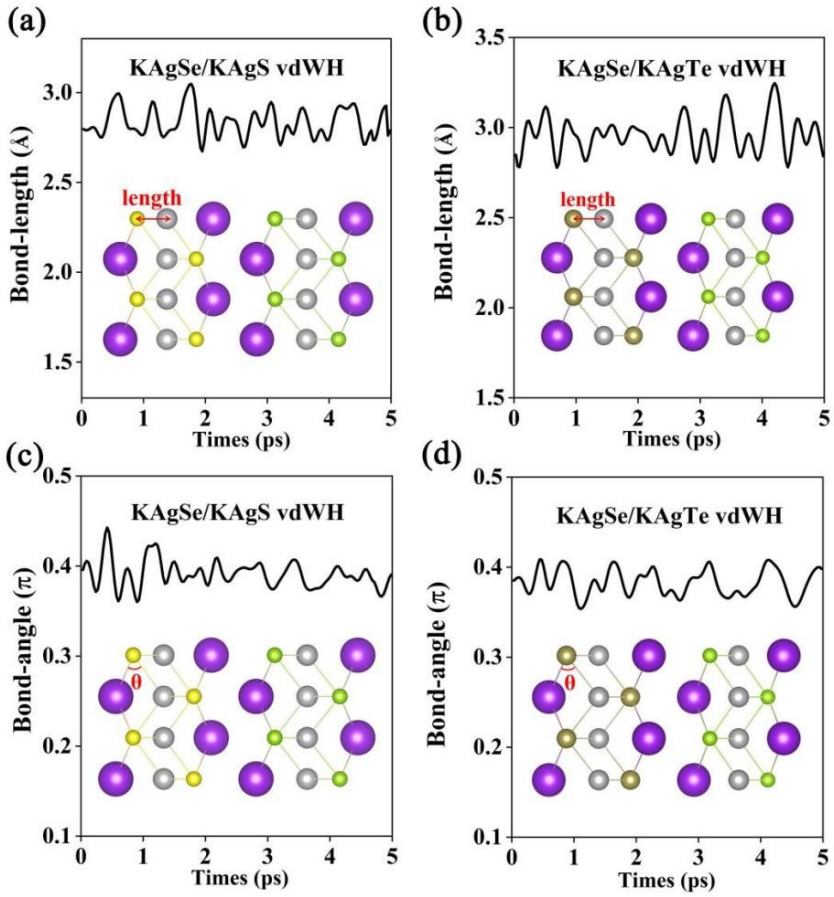

Fig. S4 The bond lengths (a-b) and angles (c-d) during the evolution process for KAgSe/KAgX vdWHs at 300 K, respectively.

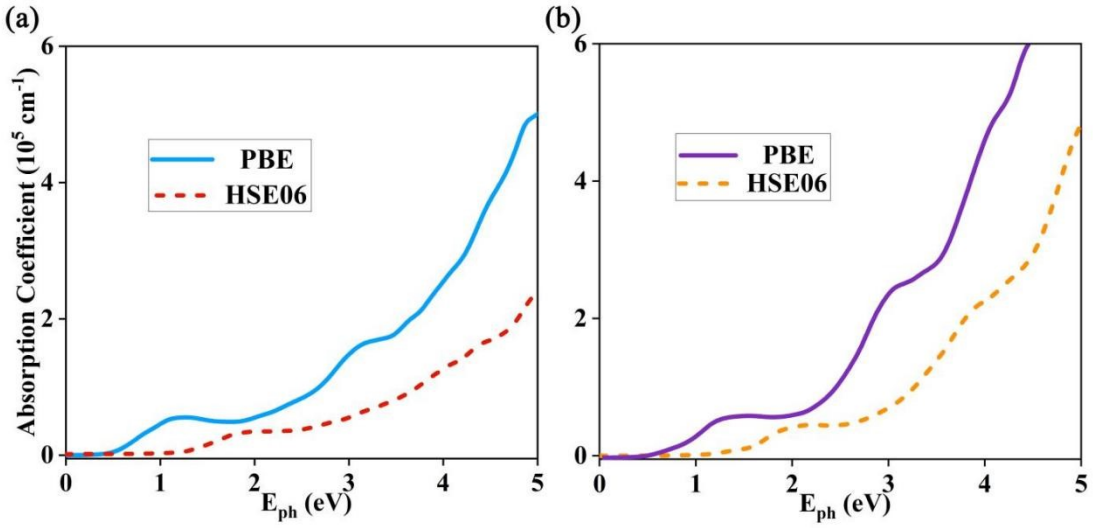

Fig. S5 Optical absorption coefficients curve upon energy of the incident light under PBE and HSE06 levels for KAgSe/KAgS (a) and KAgSe/KAgTe (b) vdWHs, respectively.