Supplementary information

The versatile characteristics of Ars/SGaInS van der Waals heterostructures

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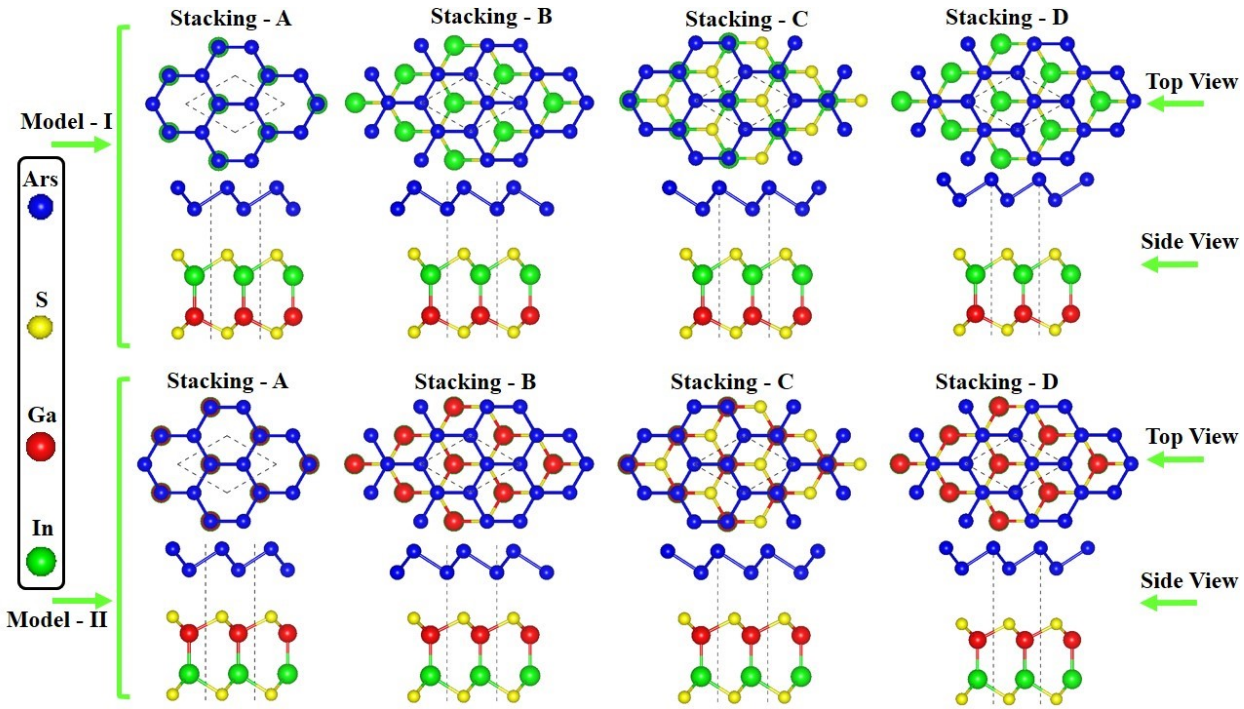

Fig. S1 An optimized top and side view of the Model-I and Model-II Ars/SGaInS vdWHs with four possible stackings (A, B, C, D).

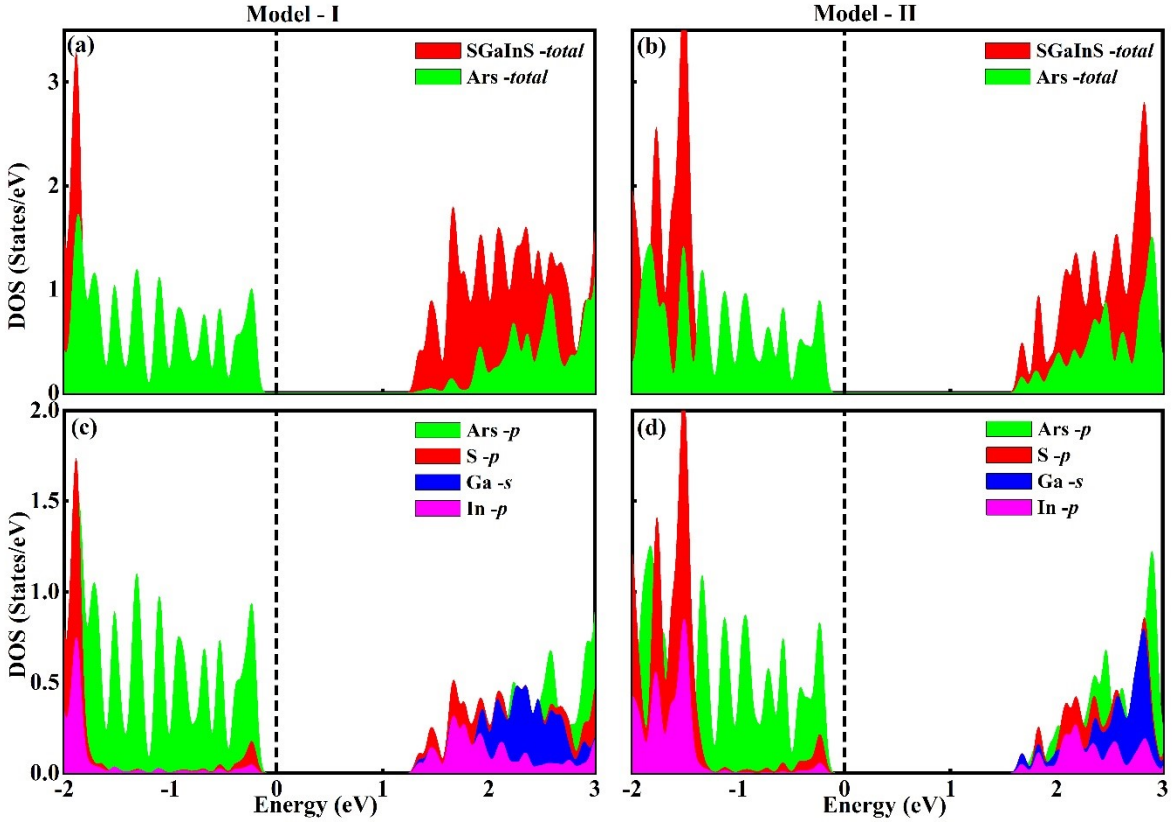

Fig. S2 Density of states of Ars/SGaInS Model-I (left column) and Model-II (right column).

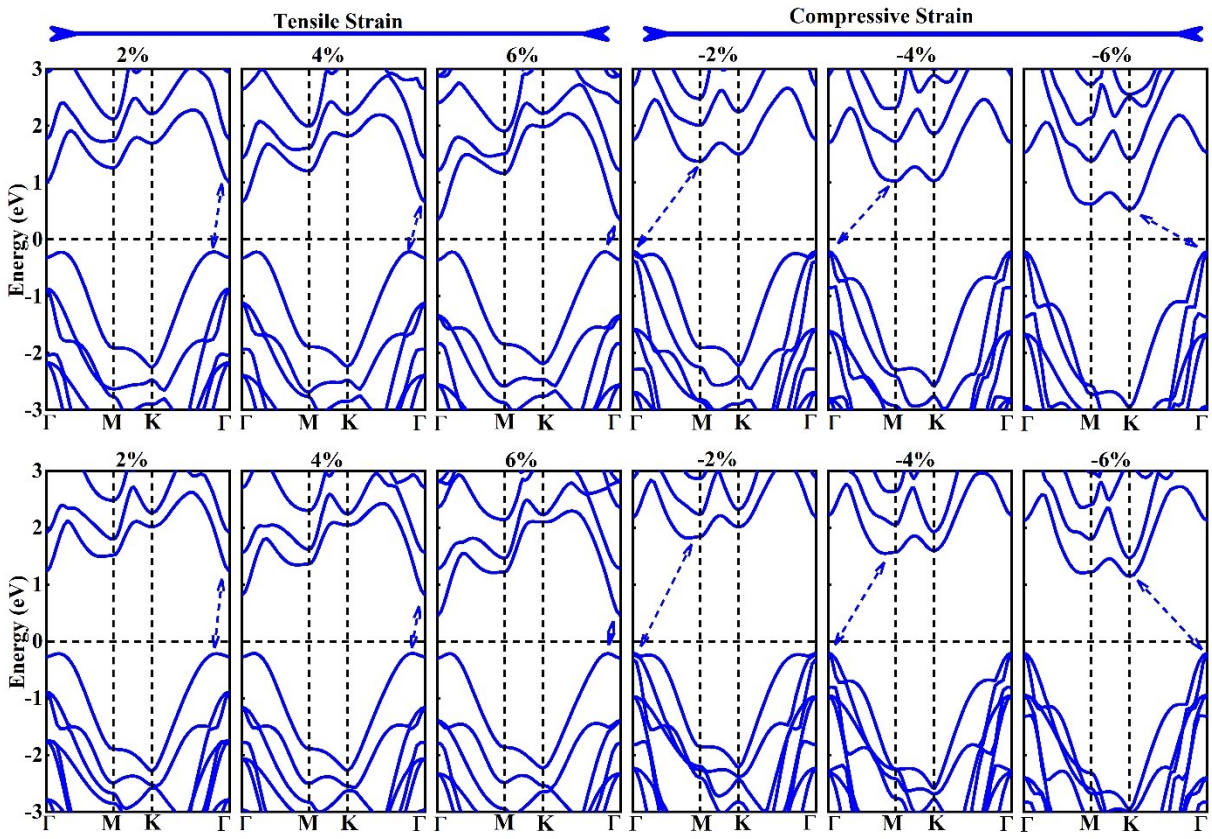

Fig. S3 Electronic band structures under tensile (2%, 4%, 6%) strain and compressive (-2%, -4%, -6%) strain of Model-I (upper panel) and Model-II (lower panel) Ars/SGaInS vdWHs.

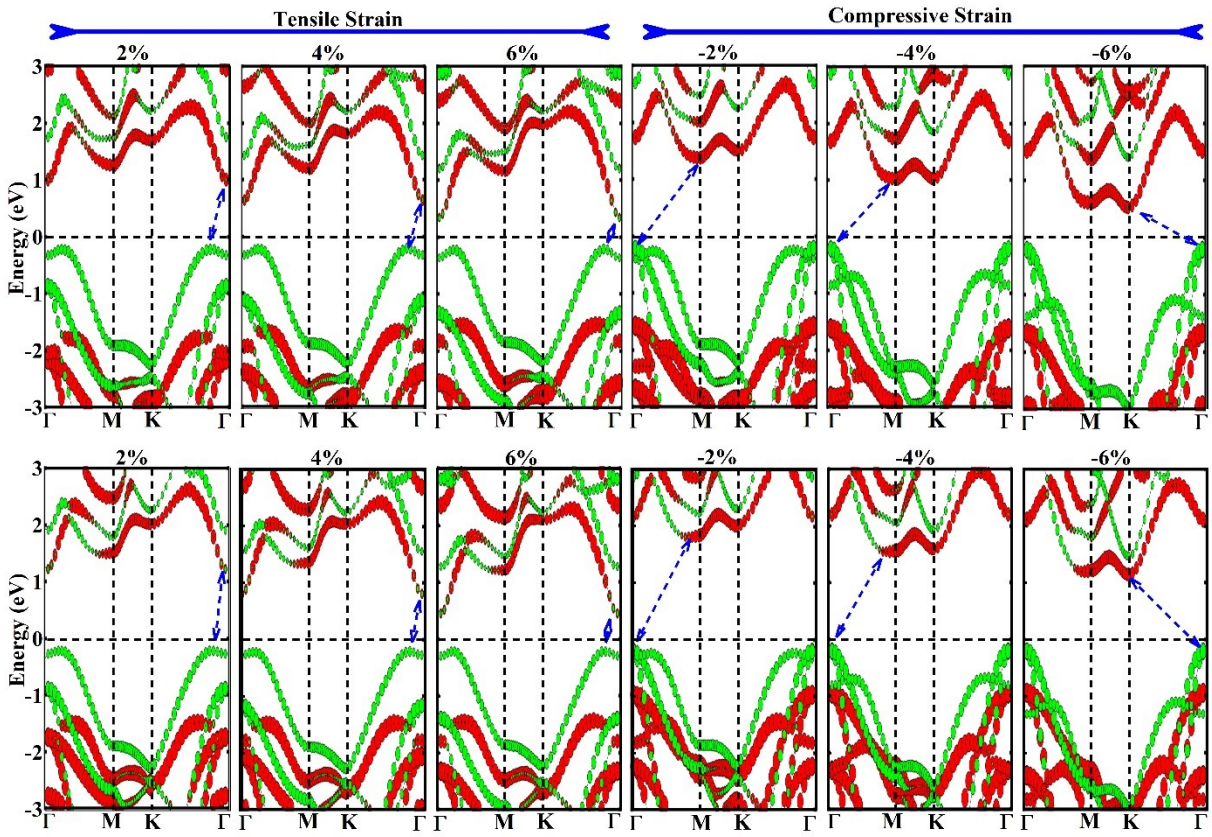

Fig. S4 Projected band structures under tensile (2%, 4%, 6%) strain and compressive (-2%, -4%, -6%) strain of Model-I (upper panel) and Model-II (lower panel) Ars/SGaInS vdWHs.

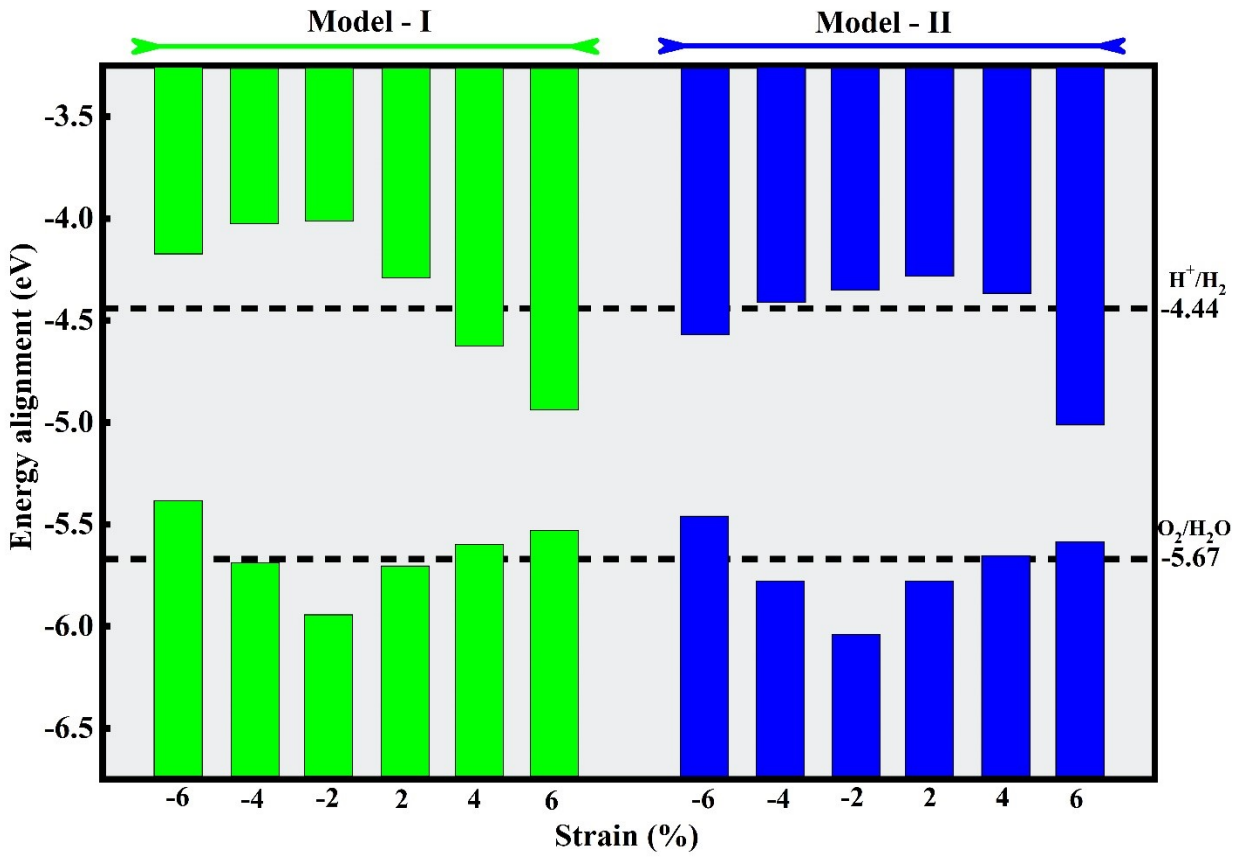

Fig. S5 The band edge positions variations under tensile (2%, 4%, 6%) strain and compressive (-2%, -4%, -6%) strain of Ars/SGaInS vdWHs Model-I and Model-II.

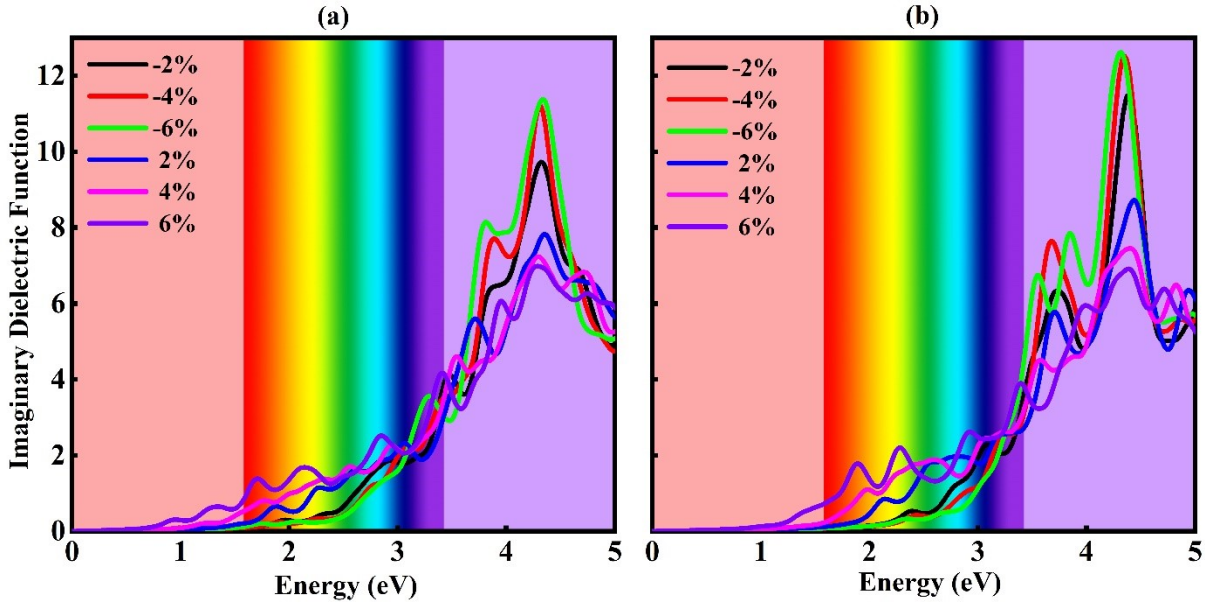

Fig. S6 The imaginary dielectric function under tensile (2%, 4%, 6%) strain and compressive (-2%, -4%, -6%) strain of Model-I (a) and Model-II (b).

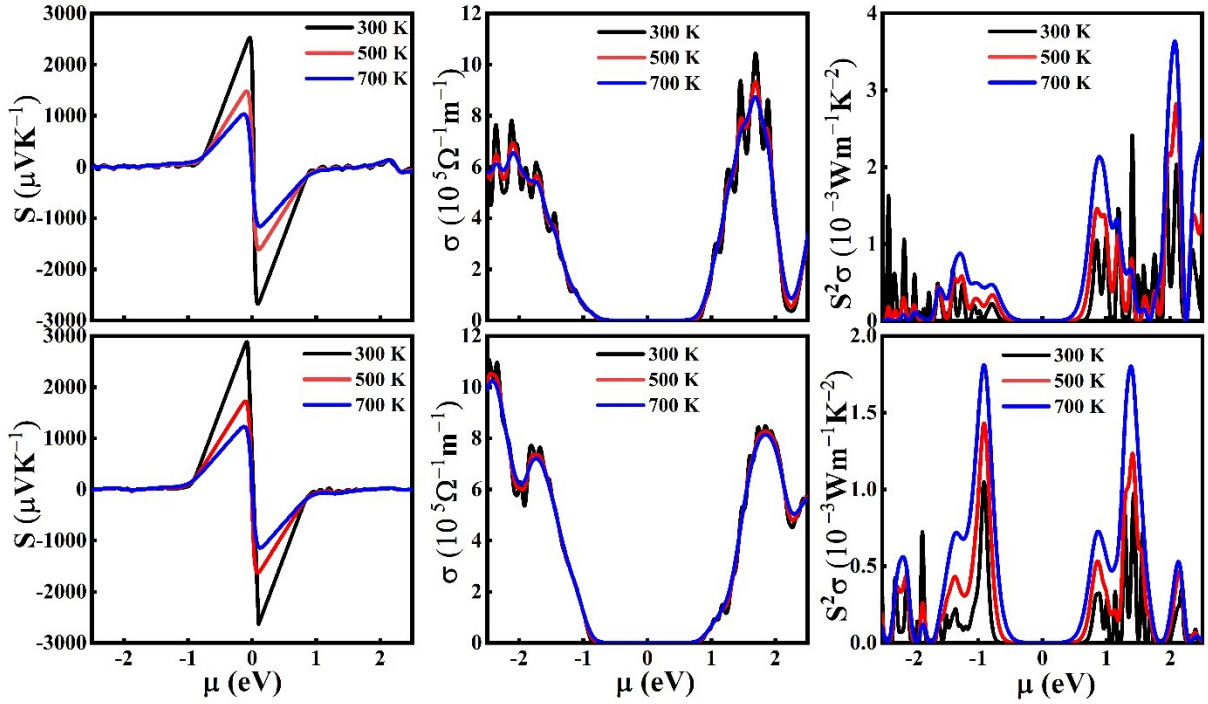

Fig. S7 The seebeck coefficient (a, b), electrical conductivity (c, d), and power factor (e, f) of Ars (upper row) and SGaInS (lower row) in relation to chemical potential.

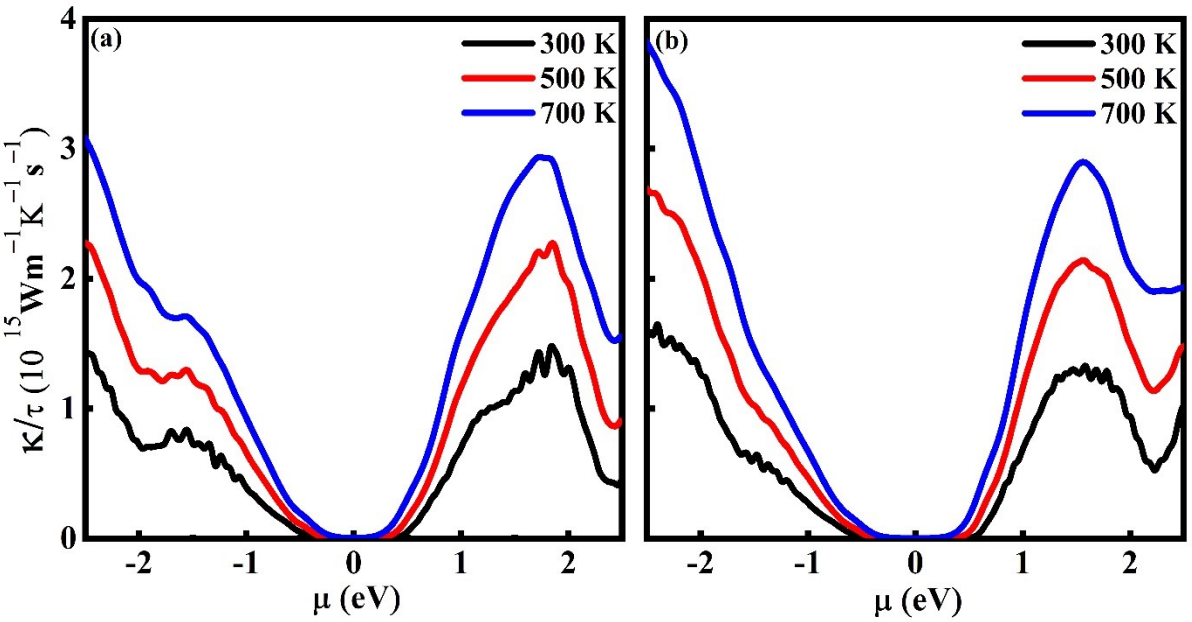

Fig. S8 Electronic thermal conductivity under 300K, 500K, and 700K temperature of Model-I (a) and Model-II (b) with respect to chemical potential.