Supplementary material

Tunable electronic properties of arsenene/GaS van der Waals heterostructures

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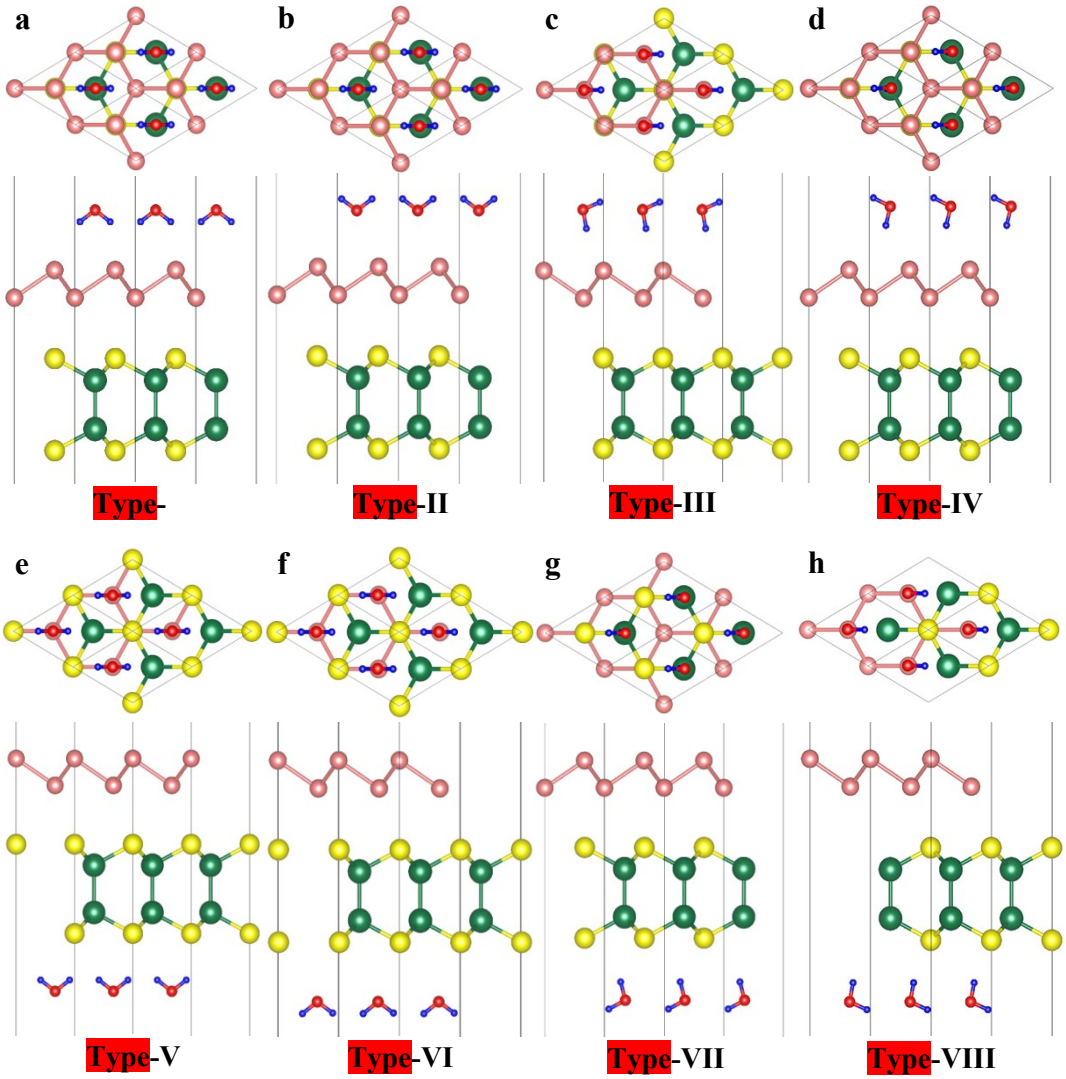

Fig. S1. (Color online) Different water adsorption configurations considered. The two-leg structures (a, b, e, f) and one-leg structures (c, d, g, h) are shown from the above (or bottom) and side. Here, “two-leg” means that the two hydrogen atoms are equidistant from the surface, while “one-leg” means that one of the two OH bonds directs the surface.[Ref.37]

Table S1. Calculated adsorption energy E_{ads} and height d (water-surface perpendicular distance) for the different adsorption configurations (see Fig. S1). The adsorption energy is defined as $E_{ads} = E_{water/heterostructure} - E_{water} - E_{heterostructure}$, where $E_{water/heterostructure}$, $E_{heterostructure}$, and E_{water} are the total energies of the water-heterostructure system, clean heterostructure, and the isolated water molecule, respectively [Ref.37]. Note that the Type-III configuration has the lowest adsorption energy.

Configuration	Type-I	Type-II	Type-III	Type-IV	Type-V	Type-VI	Type-VII	Type-VIII
E_{ads} (eV)	-0.133	-0.108	-0.323	-0.319	-0.094	-0.072	-0.291	-0.295
H/O-surface	As-H	As-O	As-H	As-H	S-H	S-O	S-H	S-H
d (Å)	2.42	2.79	2.15	2.24	2.53	2.96	2.24	2.13

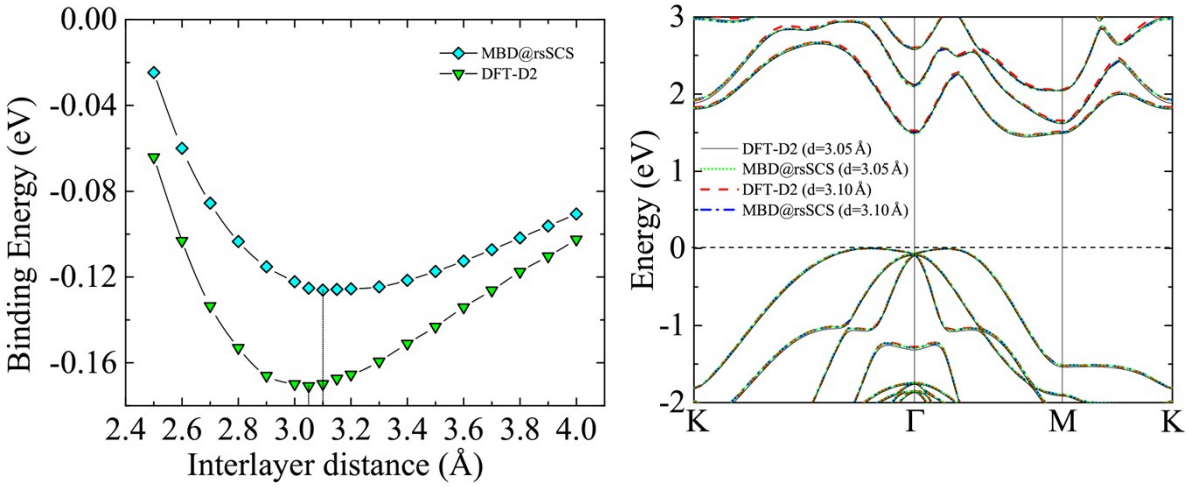

Fig.S2. (Color online) (a) Binding energies as functions of the interlayer distance and (b) band structures given by different vdW corrections: DFT-D2 and MBD@rsSCS.