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Supplementary Information

Formation of arsenene p-n junctions via organic molecular adsorption

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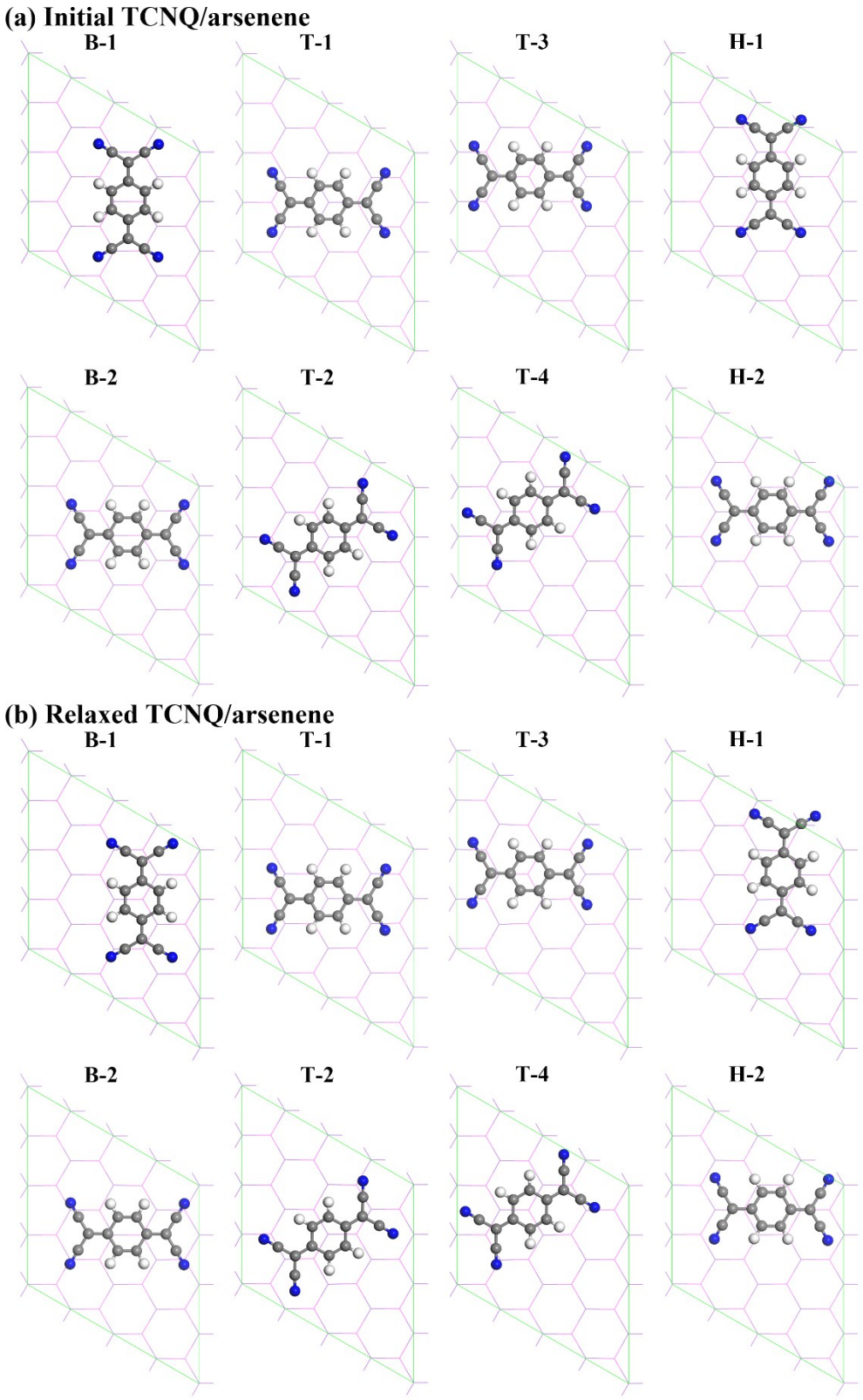

Fig. S1 Top views of the (a) initial possible configurations and (b) relaxed configurations for TCNQ/arsenene. The different sublattices of As atoms in arsenene are colored differently. N, C and H atoms are colored by blue, grey and white, respectively.

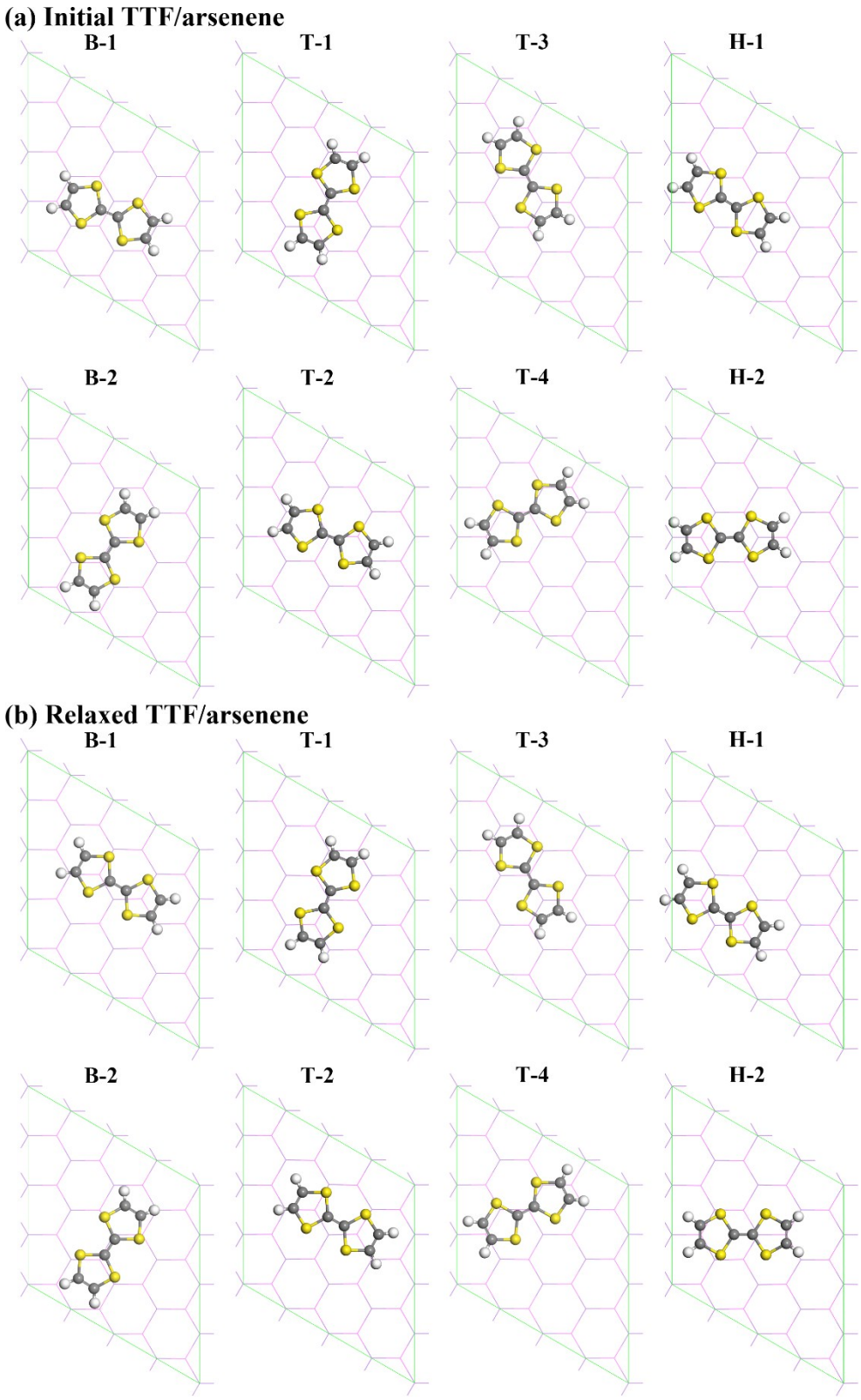

Fig. S2 Top views of the (a) initial possible configurations and (b) relaxed configurations for TTF/arsenene. The different sublattices of As atoms in arsenene are colored differently. S atoms are colored by yellow.

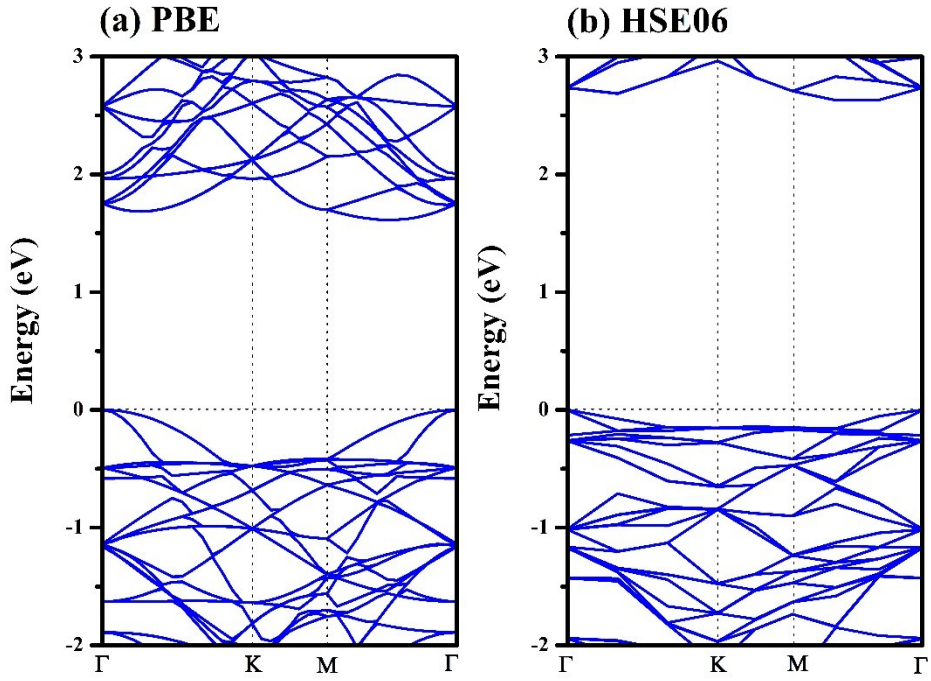

Fig. S3 Electronic band structures of arsenene monolayer calculated by (a) PBE and (b) HSE06 approaches.

Table S1: Adsorption Energies (E_{ad}), Distances between the centroid of molecule and the arsenene layer (d), and band gaps (E_p or E_n) of eight high symmetry adsorption configuration for TCNQ/arsenene and TTF/arsenene systems.

adsorbate		B-1	B-2	T-1	T-2	T-3	T-4	H-1	H-2
TCNQ	E_{ad} (eV)	1.433	1.372	1.337	1.369	1.345	1.431	1.391	1.360
	d (Å)	3.357	3.365	3.430	3.436	3.409	3.362	3.426	3.382
	E_p (eV)	0.376	0.374	0.376	0.361	0.353	0.373	0.374	0.389
TTF	E_{ad} (eV)	1.111	0.959	0.973	1.118	0.968	0.890	1.120	1.063
	d (Å)	3.329	3.512	3.417	3.325	3.412	3.383	3.325	3.099
	E_n (eV)	0.996	0.998	0.983	1.001	0.972	1.012	1.000	1.083