Electronic Supplementary Information (ESI)

Monolayer hexagonal arsenene with tunable electronic structures and magnetic properties *via* impurity doping

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1. Electronic States with Different Magnetic Moments

In order to determine the magnetic moments of the ground states of hAs, x-substituted hAs (x= B, C, N, O, Ga, Ge, Se, and monovacancy), and x-adsorbed hAs (x=As), total energies for each systems with the magnetic moments of 0.0, 1.0, 2.0, 3.0, and 4.0 μ_B were calculated with the GGA/PBE functional. From the Table S1 one can see that the ground states of the pristine, B-substituted, N-substituted, O-substituted, Ga-substituted, Se-substituted, and monovacancy-substituted hAs possess zero magnetic moment, and those of C-substituted, Ge-substituted, and As-adsorbed hAs have the magnetic moments of 1.0, 1.0, and 3.0 , respectively.

Table S1. Relative energy of electronic states with different magnetic moments (M) for hAs, x-substituted hAs (x= B, C, N, O, Ga, Ge, Se, and monovacancy), and x-adsorbed hAs (x=As). The units of relative energy and magnetic moment are eV and μ_B, respectively.

M	B-substituted hAs	C-substituted hAs	N-substituted hAs	O-substituted hAs	Ga-substituted hAs	Ge-substituted hAs	hAs	Se-substituted hAs	Monovacancy-hAs	As-adsorbed hAsA
0.0	0.000	0.139	0.000	0.000	0.000	0.113	0.000	0.000	0.000	0.152
1.0	0.711	0.000	0.738	0.063	0.599	0.000	0.859	0.045	0.035	0.116
2.0	1.418	0.884	1.556	1.246	1.237	0.907	1.841	0.943	0.359	0.055
3.0	2.292	1.844	2.426	2.171	2.118	1.888	2.875	1.899	0.674	0.000
4.0	3.221	2.847	3.349	3.148	3.090	2.892	3.958	2.898	1.643	0.938

2. Band Structures of the Doped hAs with 6×6 Supercell

In order to evaluate the influences of the size of supercell on electronic structures of the doped systems, the test calculations of band structures of the supercell with 6×6 were performed for the B-, Ga-, O-, and Se-substituted hAs. Among all substitutional atoms, B and Ga possess large atomic radius and O and Se have strong electronegativity. In the 6×6 supercell, the distance between two neighboring doping atom is increased up to 21.5 Å. As shown in Fig. S1, compared with those of the doped systems with the 4×4 supercell, the main results remain unchanged although the band bending become a little slight.

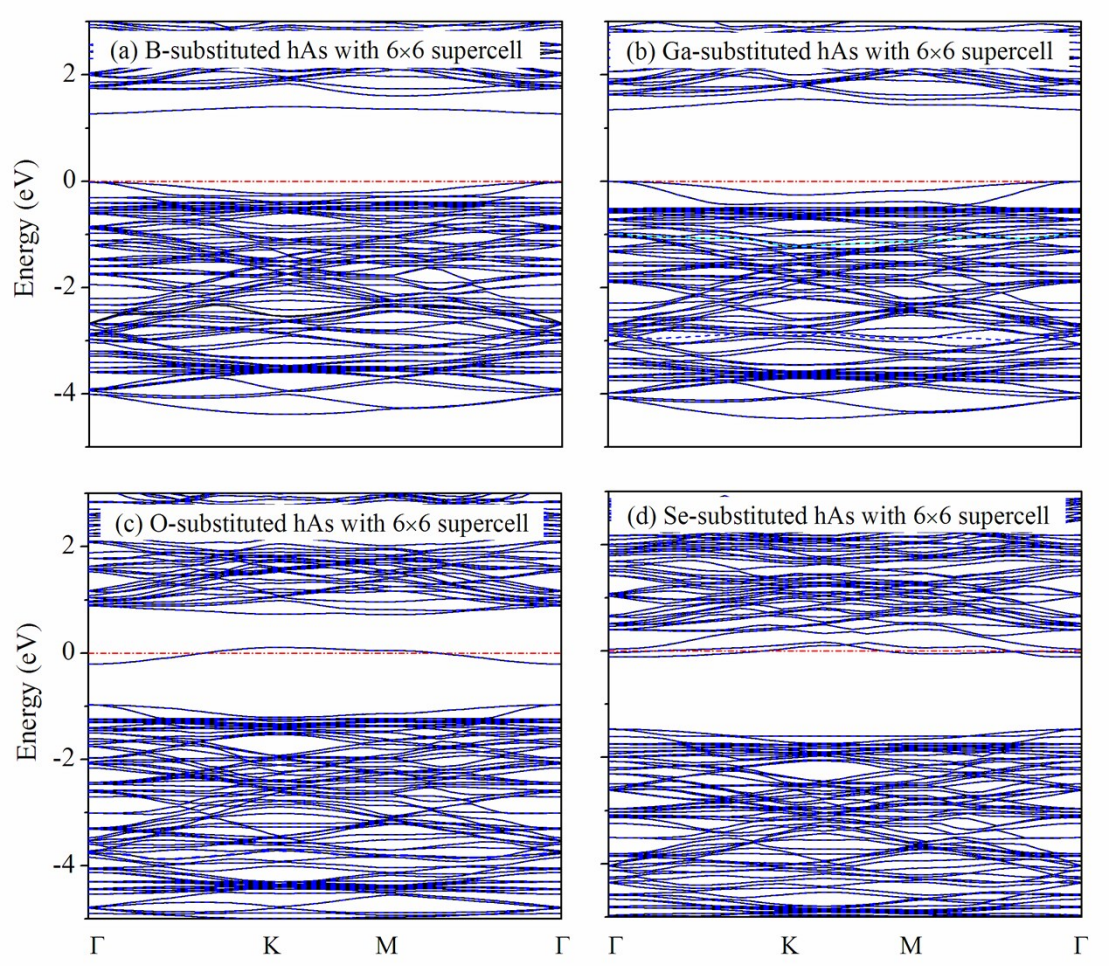

Fig. S1 Spin-polarized band structures of (a) B-substituted, (b) Ga-substituted, (c) O-substituted, and (d) Se-substituted hAs. Black solid and blue dashed lines denote spin-up and spin-down channels and red dash-dot lines indicate the Fermi level, respectively.

3. Band Structures of the Doped hAs with Spin-Orbit Coupling Effects

To evaluate the spin-orbit coupling (SOC) effects on electronic structures, the band structures of the studied systems were calculated by non-collinear calculations implemented in VASP. Compared with those without SOC, the band structures with SOC show few changes, as shown in Fig. S2 and S3.

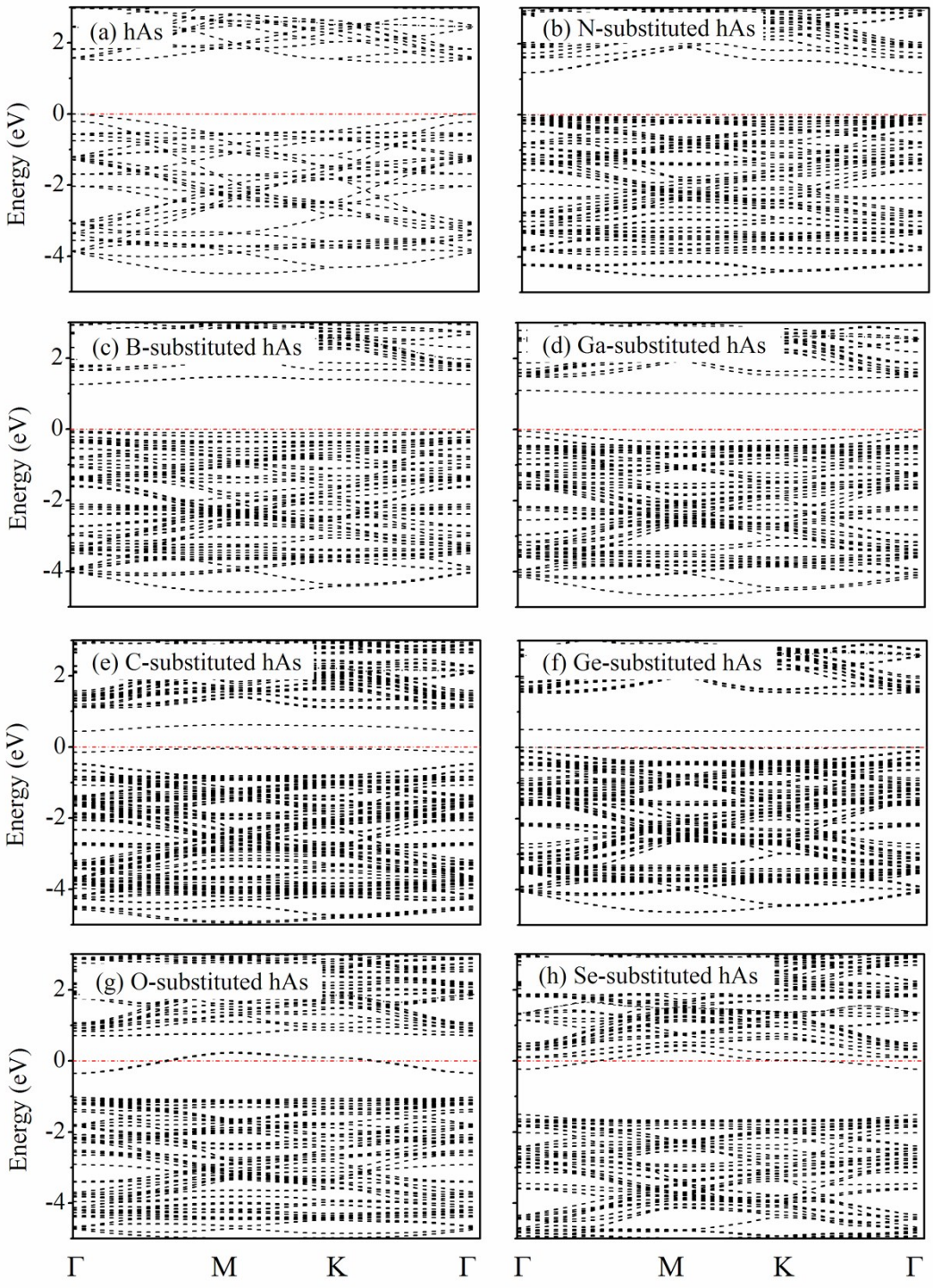

Fig. S2 Band structures with spin-orbit coupling effects for (a) hAs, (b) N-, (c) B-, (d) Ga-, (e) C-, (f) Ge-, (g) O-, and (h) Se-substituted hAs. Red dash-dot lines indicate the Fermi level.

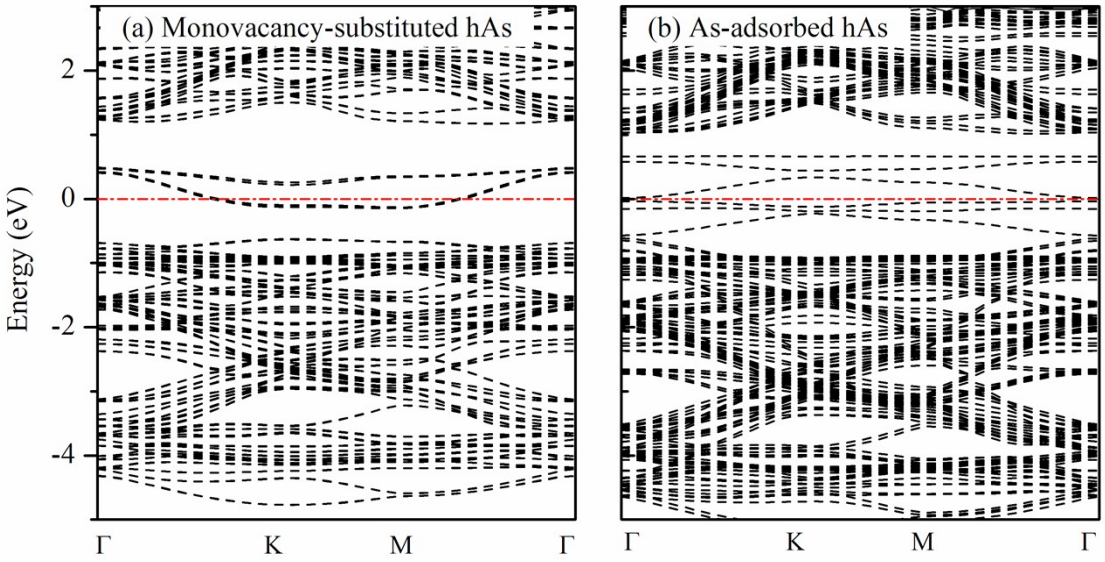

Fig. S3 Band structures with spin-orbit coupling effects for (a) monovacancy-substituted, and (b) As-adsorbed hAs. Red dash-dot lines indicate the Fermi level.

4. Band Structures of the pristine hAs

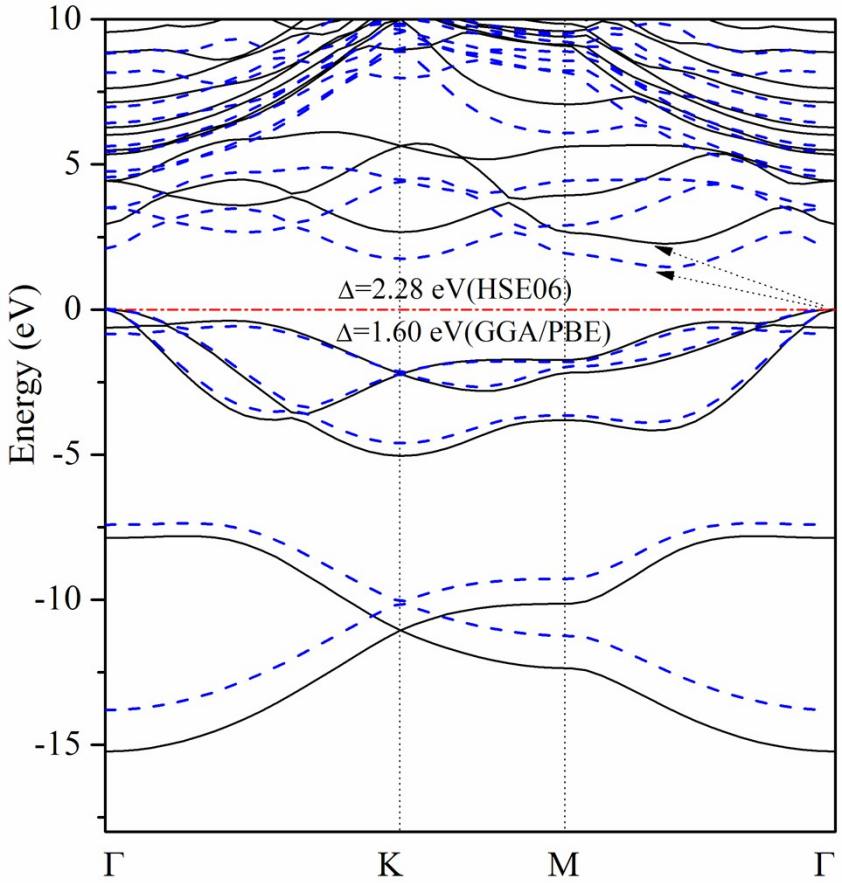

Fig. S4 Band structure of pristine hAs. Black solid and blue dashed lines denote results calculated at HSE06 and GGA/PBE levels, respectively. Red dash-dot line indicates the Fermi level.