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Supporting Information

Novel electronic and optical properties in ultrathin Silicene/Arsenene heterostructures and electric field effects

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Calculation of in-plane stiffness and Poisson's ratio for arsenene

To calculate the elastic constants of arsenene, the strain is applied in a rectangular unit cell, as depicted in Figure S1(a). a_x and a_y are the lattice constants along the x and y directions. By changing the lattice constant a with strain ε in the harmonic region, namely, $a \rightarrow a+a\cdot\varepsilon$, the strained arsenene is obtained. The strain ε_x and ε_y are applied along the two lattice vector directions, respectively, ranging from -0.008 to 0.008 for each direction, with an increment $\Delta\varepsilon$ of 0.002. Thus, we get a mesh grid containing 81 data points. For each grid point, the corresponding atomic structure of the unit cell is fully reoptimized and their total energy is obtained, as shown Figure S1(b). Also, no reconstructures occur due to the small strain. Then, by using the polynomial fitting method, the strain energy (E_S) is fitted by the formula: $E_S = a_1\varepsilon_x^2 + a_2\varepsilon_y^2 + a_3\varepsilon_x\cdot\varepsilon_y$. The in-plane stiffness of the material along the x and y directions are expressed as $C_x = (2a_1 - a_3^2/2a_2)/A_0$ and $C_x = (2a_2 - a_3^2/2a_1)/A_0$, where A_0 is the equilibrium area of the unit cell. The Poisson's ratio of the material along x and y directions are equal to $\nu_x = a_3/2a_2$ and $\nu_y = a_3/2a_1$, respectively. As a result, a fitted quadratic polynomial $E_S = 36.75\varepsilon_x^2 + 36.68\varepsilon_y^2 + 13.08\varepsilon_x\cdot\varepsilon_y$ is obtained. The fitted surface plot of the total energy varying with strains is presented in Figure S1(c). Therefore, the calculated in-plane C (ν) are 50.6 N/m (0.178) in the x direction and 50.46 N/m (0.178) in the y direction, which means that arsenene is an isotropy material.

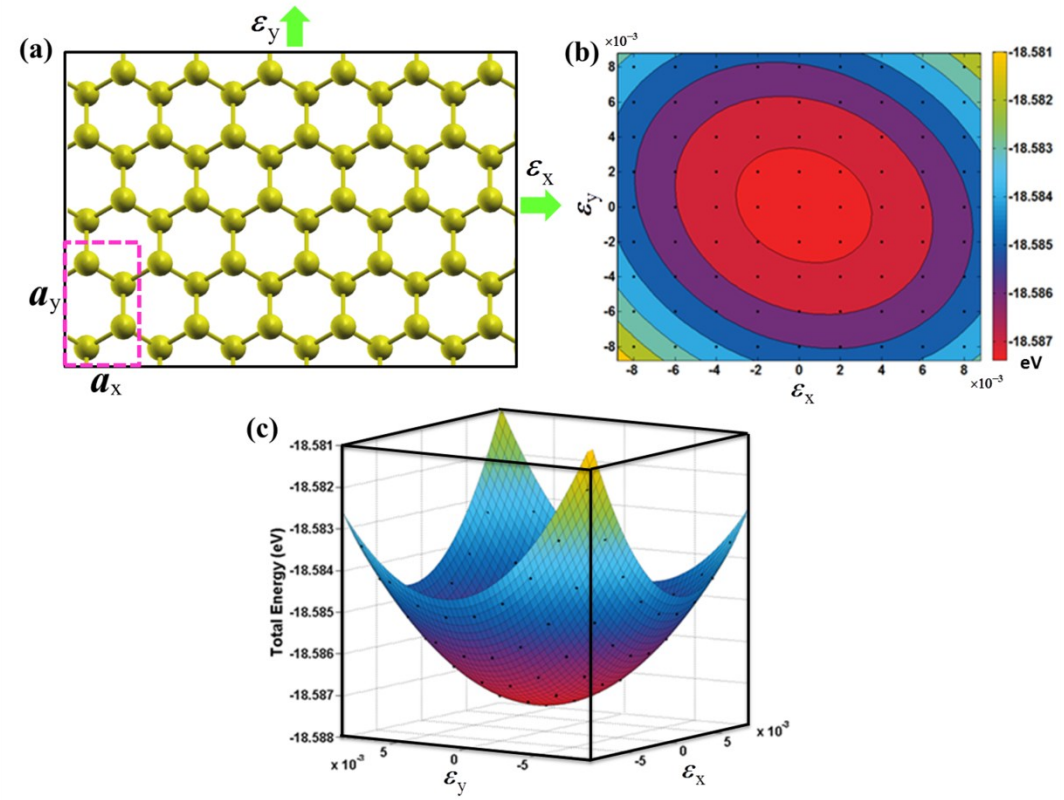

Figure S1. (a) The atomic structure of monolayer arsenene. The rectangular cell used for elastic constants calculation is shown by the pink dashed line. a_x and a_y are the lattice constants. The contour (b) and three-dimensional fitted surface (c) plot of the total energy versus strain.

Table S1: The calculated 2D in-plane stiffness (C), Poisson's ratio (v), and effective mass (m*) in the zigzag and armchair directions of AA- and AB-stacking.

System	Direction	C (N·m^{-1})	v	m* (m_e)
AA	zigzag	86.6	0.289	0.059 (e)
				0.057 (h)
	armchair	86.6	0.288	0.058 (e)
				0.055 (h)
AB	zigzag	95.7	0.325	0.024 (e)
				0.023 (h)
	armchair	95.7	0.325	0.024 (e)
				0.023 (h)

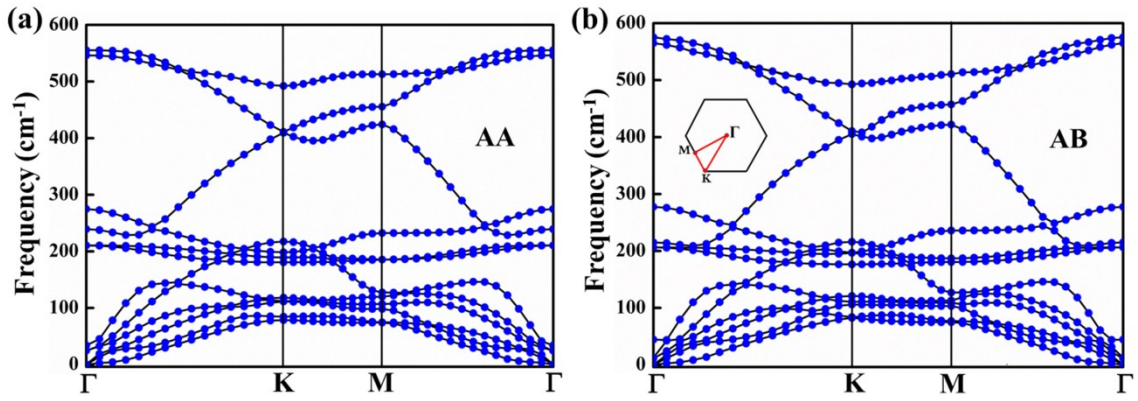

Figure S2. Phonon band dispersions of Si/As heterostructures with AA-stacking (a) and AB-stacking (b), which exhibit outstanding kinetic stability.

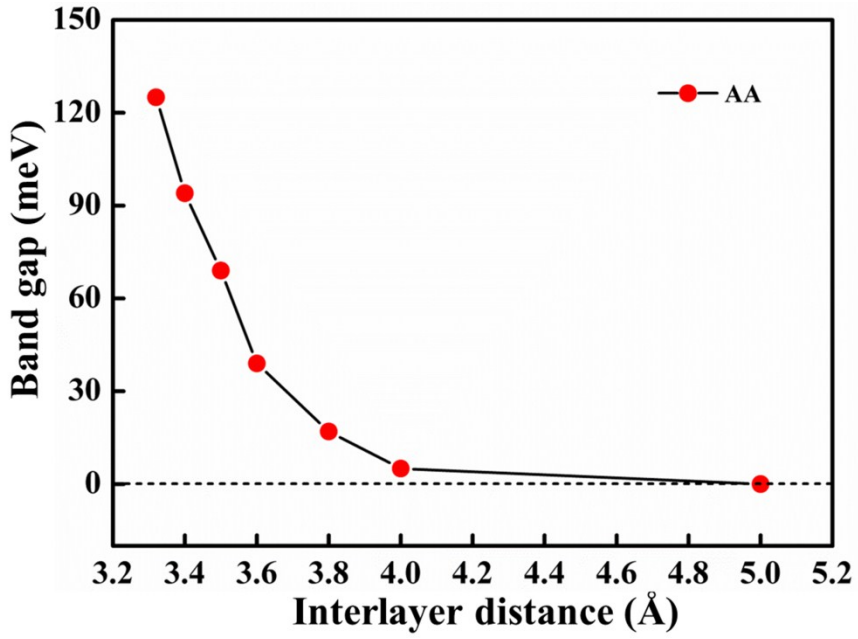

Figure S3. The variation of PBE band gap of silicene as a function of interlayer distance in AA-stacking structure.

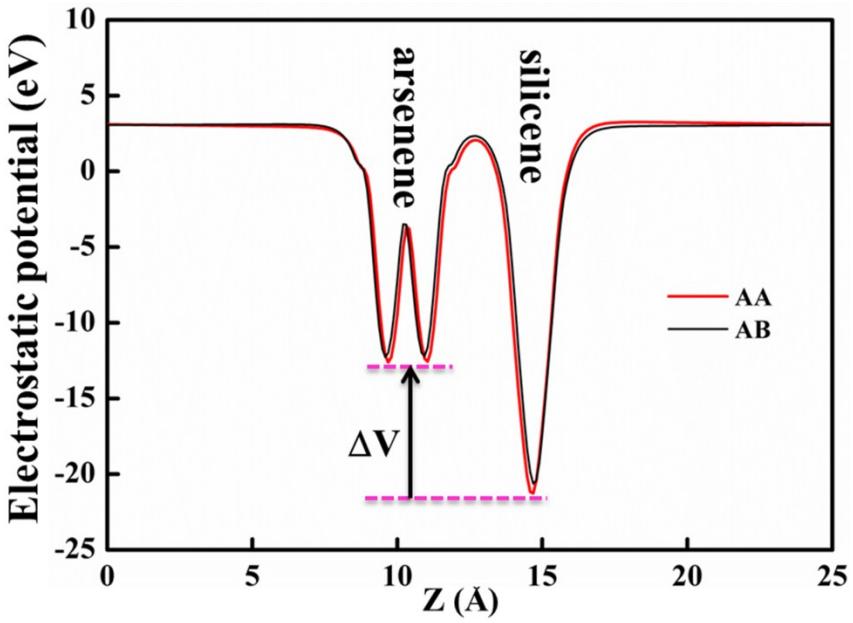

Figure S4. Electrostatic potential of the Si/As heterostructure with AA- and AB-stacking.

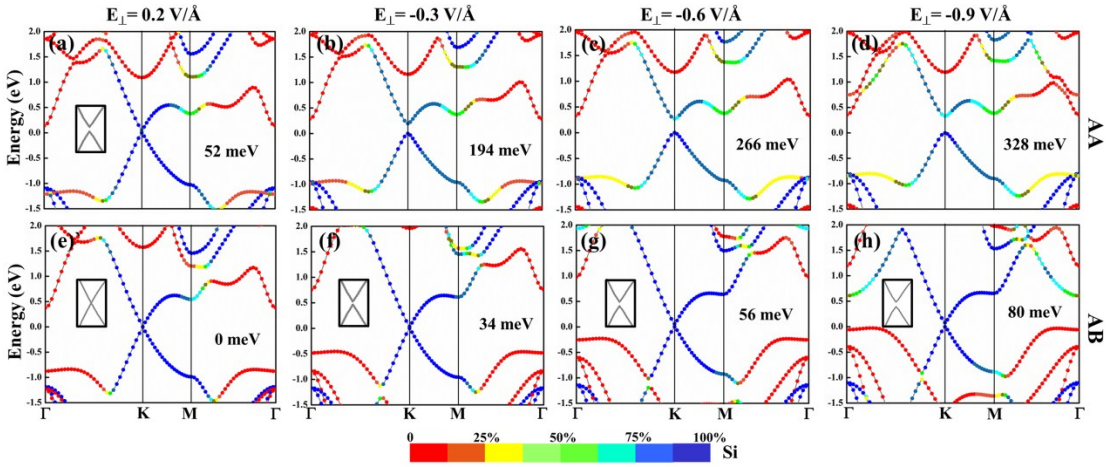

Figure S5. Projection resolved band structures of Si/As heterostructure under various external electric fields ($E_{\perp}$): AA-stacking (a-d) and AB-stacking (e-h).