Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

First principles study of BAs/$MoSi_2N_4$ van der Waals heterostructure: tunable electronic and optical properties via vertical strain

Yunxi Qi[a], Can Yao[a], Jun Zhao[a], and Hui Zeng[b]

[a]New Energy Technology Engineering Laboratory of Jiangsu Province & School of Science, Nanjing University of Posts and Telecommunications, Nanjing, Jiangsu 210023, China

[b]School of Microelectronics, Nanjing University of Science and Technology, Nanjing, Jiangsu 210094, China

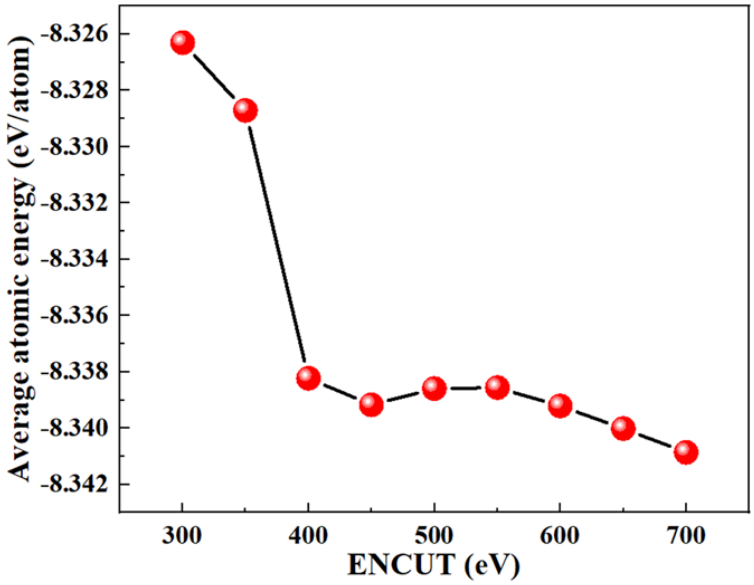

Fig. S1 Convergence test of BAs/$MoSi_2N_4$ heterostructure under different cut-off energies.

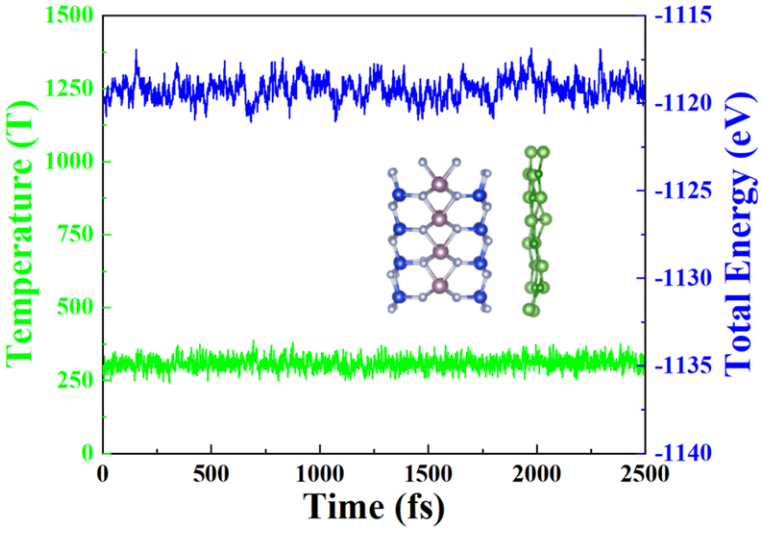

Fig. S2 The AIMD results of A_1-stacked BAs/$MoSi_2N_4$ heterostructure. The evolution

curves of total energy and temperature relative to simulation time are represented by blue and green lines, respectively. The insert shows the final snapshot of the heterostructure after 5 ps.

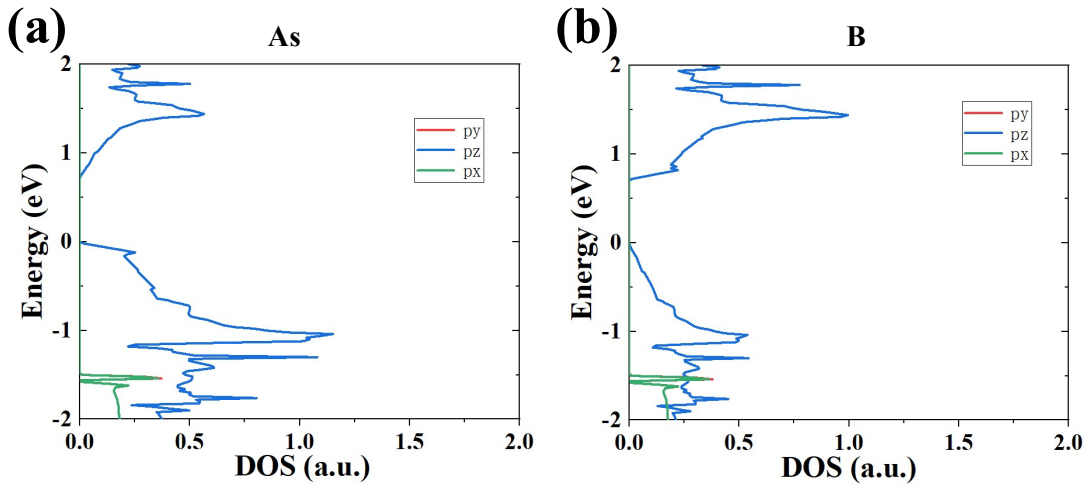

Fig. S3 The density of states of B and As atoms in the $BAs/MoSi_2N_4$ heterostructure.

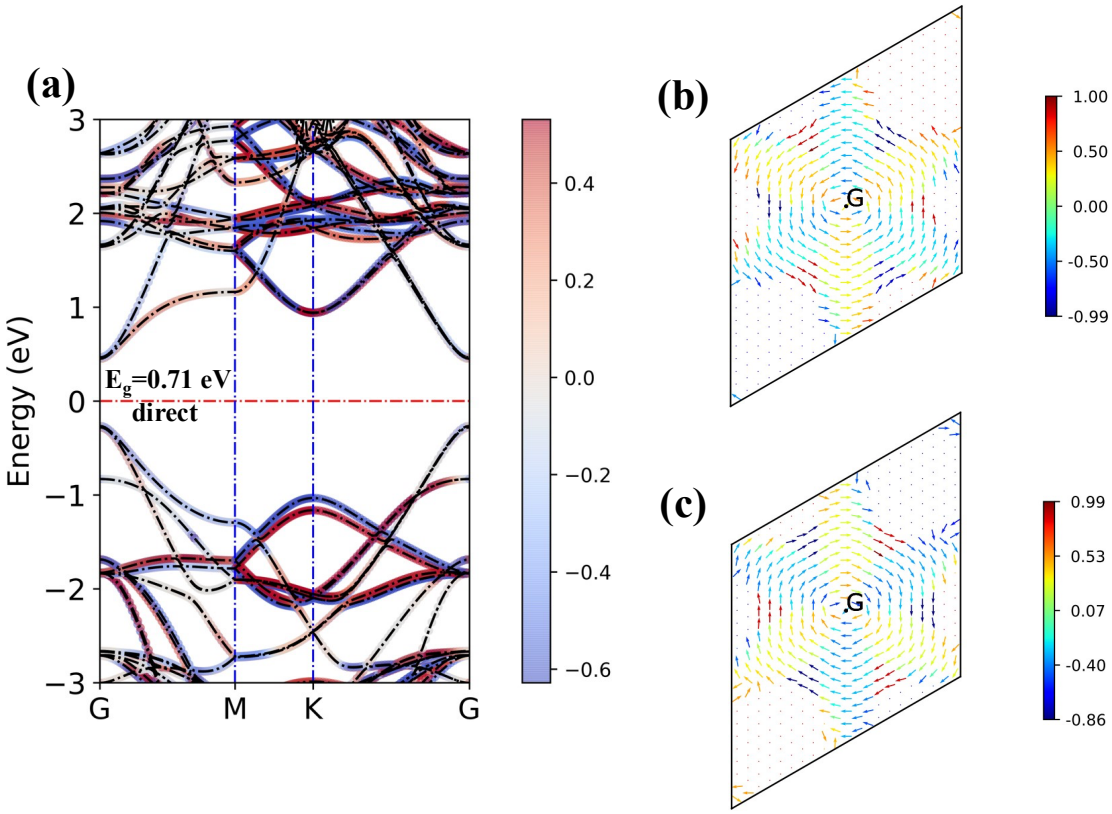

Fig. S4 The band structure of the $BAs/MoSi_2N_4$ heterostructure including SOC. Color represents the weight of S_Z in the $BAs/MoSi_2N_4$ heterostructure. The figure on the right shows the spin texture of (b) the highest occupation state and (c) the second highest occupation state near the G point in the Brillouin zone. The arrow represents the in-plane component of spin polarization, and the color represents the out of plane component of spin polarization.

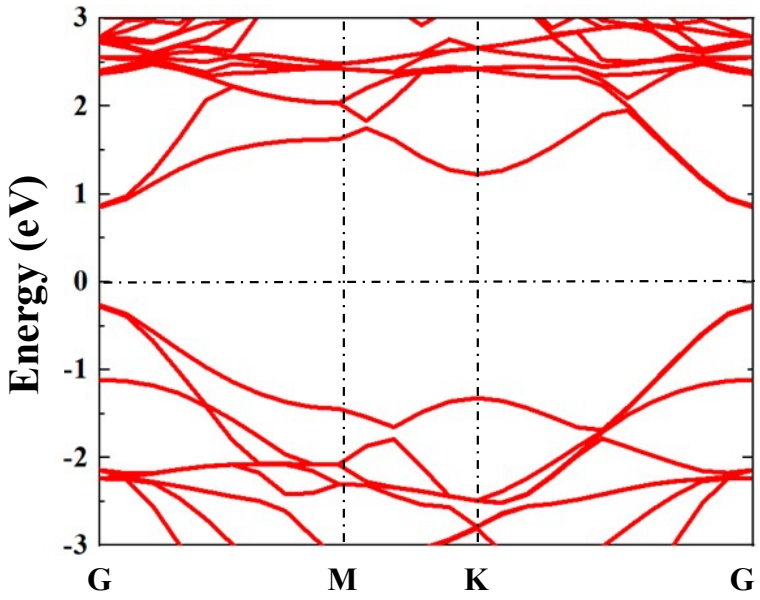

Fig. S5 HSE06 band structure of BAs/$MoSi_2N_4$ heterostructure.

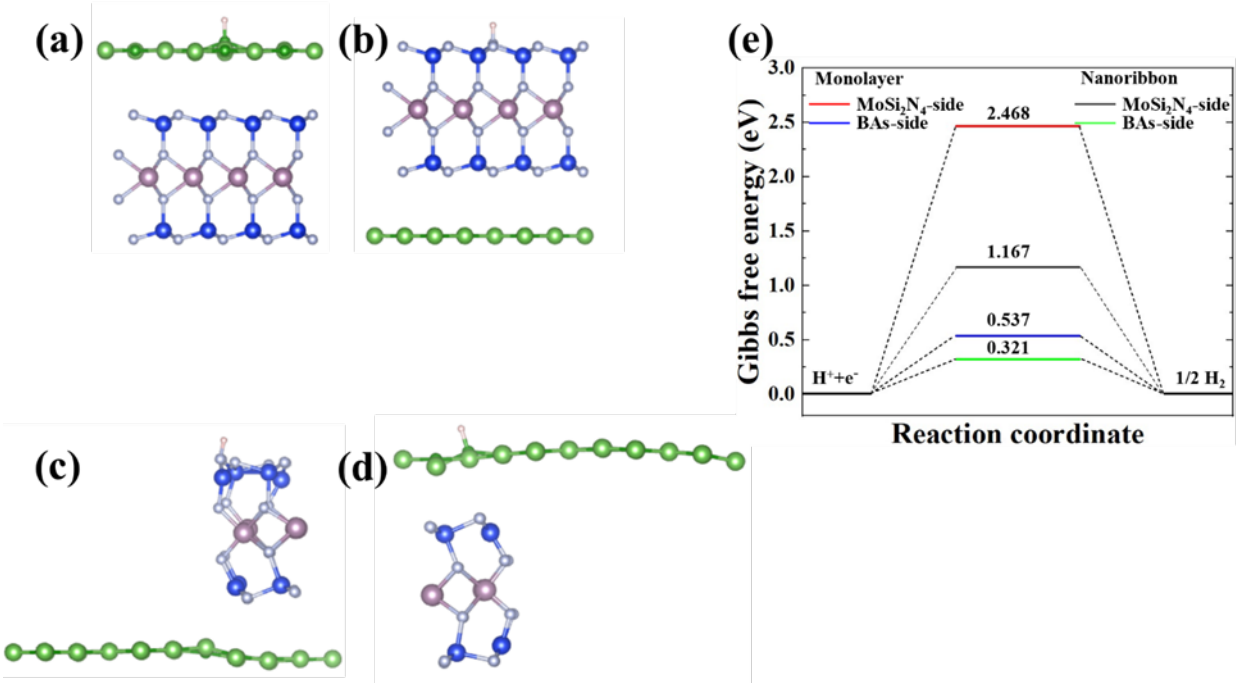

Fig. S6 (a –d) Side view of monolayer and ribbon BAs/$MoSi_2N_4$ heterostructures, with hydrogen atoms adsorbed at the most favorable positions on both sides. (e) Gibbs free energy distribution of HER on both sides of monolayer and ribbon BAs/$MoSi_2N_4$ heterostructures.

Table S1 The lattice constants a and b, equilibrium distance D, bandgap E_g, and total energy E_t of the BAs/$MoSi_2N_4$ heterostructure under different vacuum layer thicknesses.

Vacuum Layer (Å)	a = b (Å)	D (Å)	E_g (eV)	E_t (eV)
15	5.83	3.9	0.721	-283.9726
20	5.82	3.5	0.716	-283.5109
25	5.82	3.5	0.717	-283.4856