

## Supplementary Information

### Effect of external electric field on the electronic properties of AlAs/SiC van der Waals heterostructure

Zicheng Zhang,<sup>a</sup> Changxin Wan,<sup>a</sup> Heng Li,<sup>b,c</sup> Chunsheng Liu,<sup>a</sup> Lan Meng,<sup>\*a</sup> Xiaohong Yan,<sup>a</sup>

<sup>a</sup>College of Electronic and Optical Engineering & College of Flexible Electronics (Future Technology), Nanjing University of Posts and Telecommunications, Nanjing 210023, China

<sup>b</sup>Jiujiang Research Institute of Xiamen University, Jiujiang, 332000, China

<sup>c</sup>Fujian Provincial Key Laboratory of Semiconductors and Applications, Collaborative Innovation Center for Optoelectronic Semiconductors and Efficient Devices,

Department of Physics, Xiamen University, Xiamen, 361005, China

E-mail: [menglan@njupt.edu.cn](mailto:menglan@njupt.edu.cn)

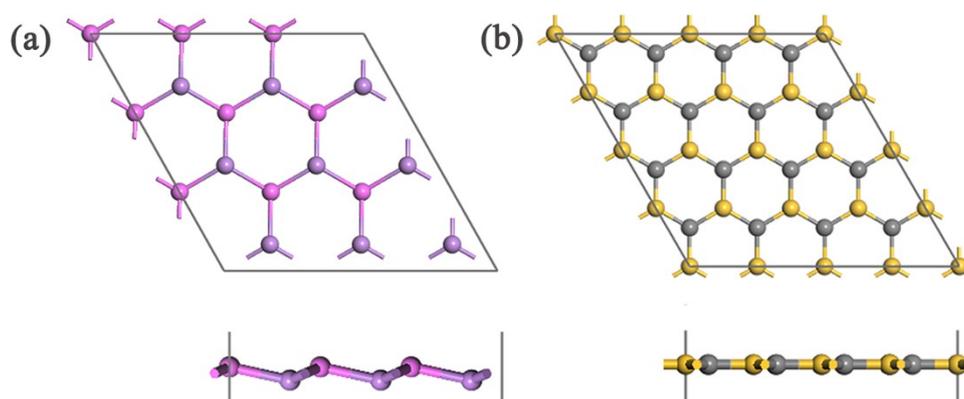


Fig. S1 The top and side views of optimized monolayer AlAs and SiC structure.

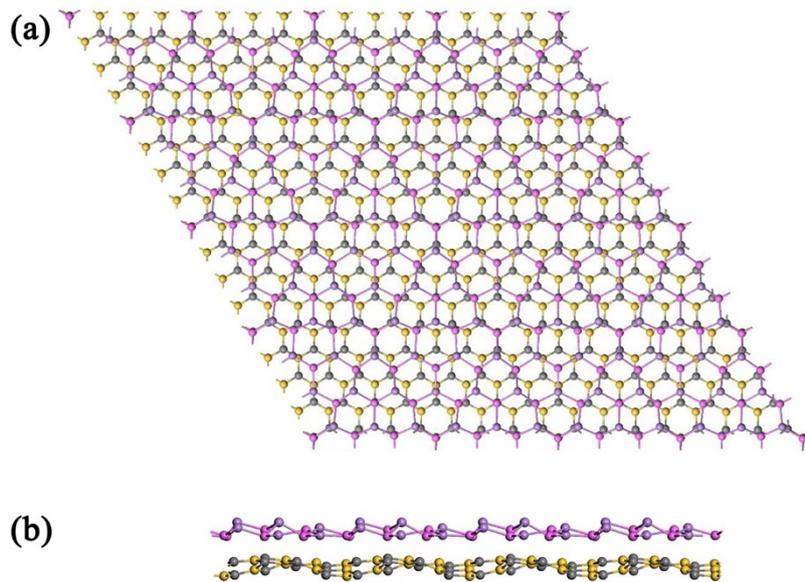


Fig. S2 The top and side views of optimized 2D AlAs/SiC heterostructure.

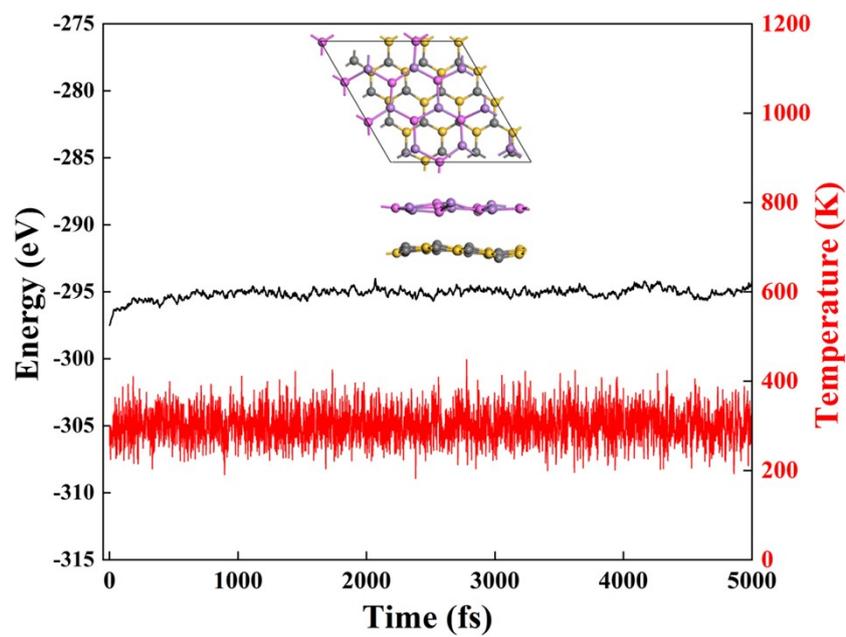


Fig. S3 AIMD simulations of AlAs/SiC heterostructure for 5 ps (5000 fs) with time step of 1fs at 300K.

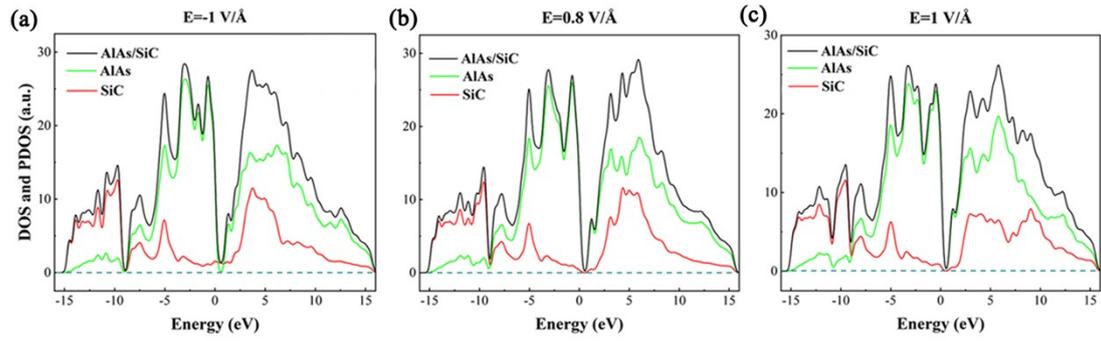


Fig. S4 DOS and PDOS of metallic AlAs/SiC heterostructure under  $-1 \text{ V/\AA}$ ,  $0.8 \text{ V/\AA}$  and  $1.0 \text{ V/\AA}$  electric fields.