

Layer-dependent photocatalysts of GaN/SiC-based multilayer van der Waals heterojunctions for Hydrogen Evolution

Bojun Peng,^{ab} Liang Xu,^{ac*} Jian Zeng,^a Xiaopeng Qi,^{b*} Youwen Yang,^a Zongle Ma,^a

Xin Huang,^a Ling-Ling Wang^c and Cijun Shuai^{ad*} □

^a Energy Materials Computing Center, School of Energy and Mechanical Engineering, Jiangxi University of Science and Technology, Nanchang 330013, China.

^b Faculty of Materials Metallurgy and Chemistry, Jiangxi University of Science and Technology, Ganzhou, 341000, China.

^c School of Physics and Electronics, Hunan University, Changsha 410082, China.

^d State Key Laboratory of High Performance Complex Manufacturing, Central South University, Changsha 410083, China.

Table S1 The interface binding energy (E_{ad}) for various GaN/SiC van der waals heterojunctions.

Structure	Interface Binding Energies (eV)			
	GaN/SiC	GaN/SiC/GaN	GaN/GaN/SiC	Bi-GaN/Bi-SiC
a	-0.52432	-1.0801325	-1.56703	-1.7399054
b	-0.34881	-1.2765097	-1.02816	-1.3834042
c	-0.55197	-1.0944155	-1.39374	
d	-0.67353	-1.2461816	-1.43105	

e	-0.36302	-1.0305702	-1.2021	
f	-0.41949	-1.5772833	-0.96721	

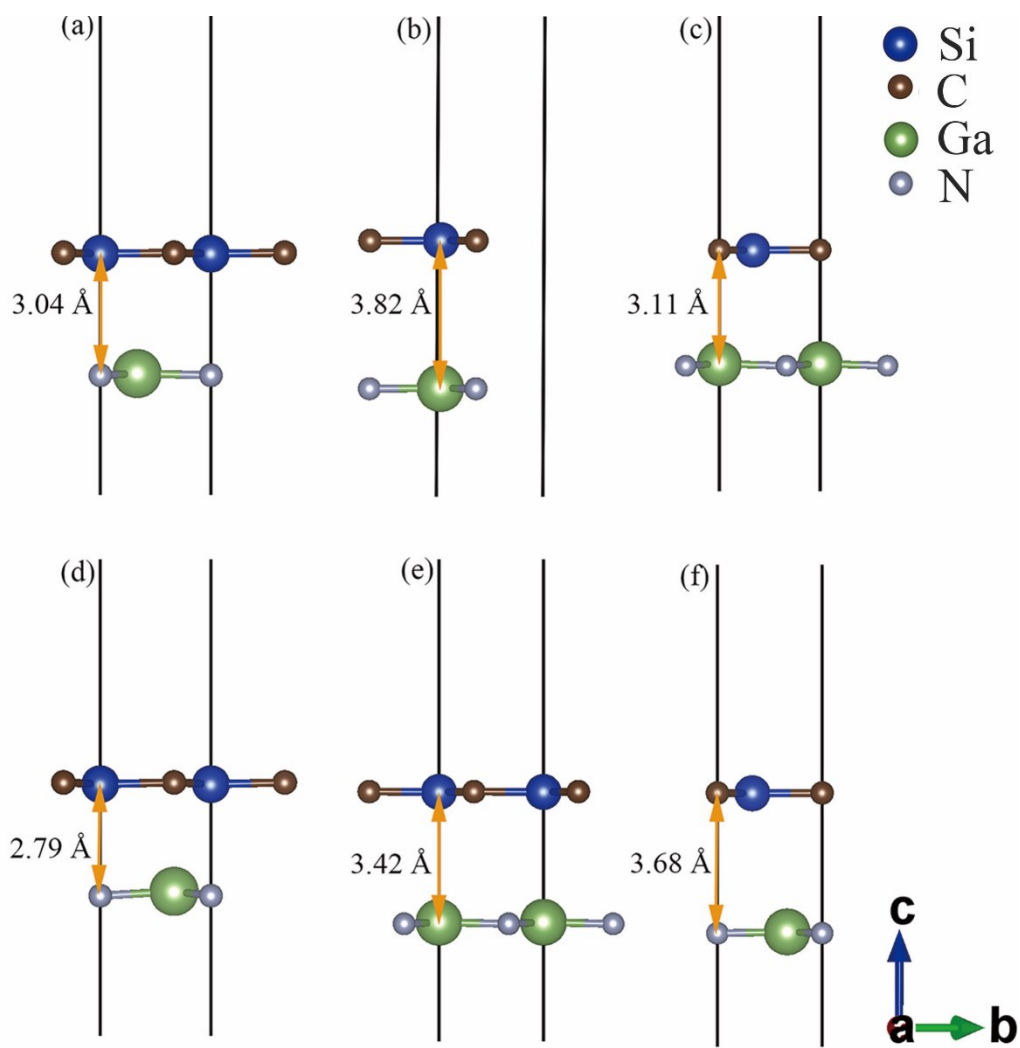


Fig. S1 Side views of the optimized structures of the GaN/SiC bilayer with different staking. The interlayer spacing (along the z axis) between the individuals of the heterojunctions are calculated and given.

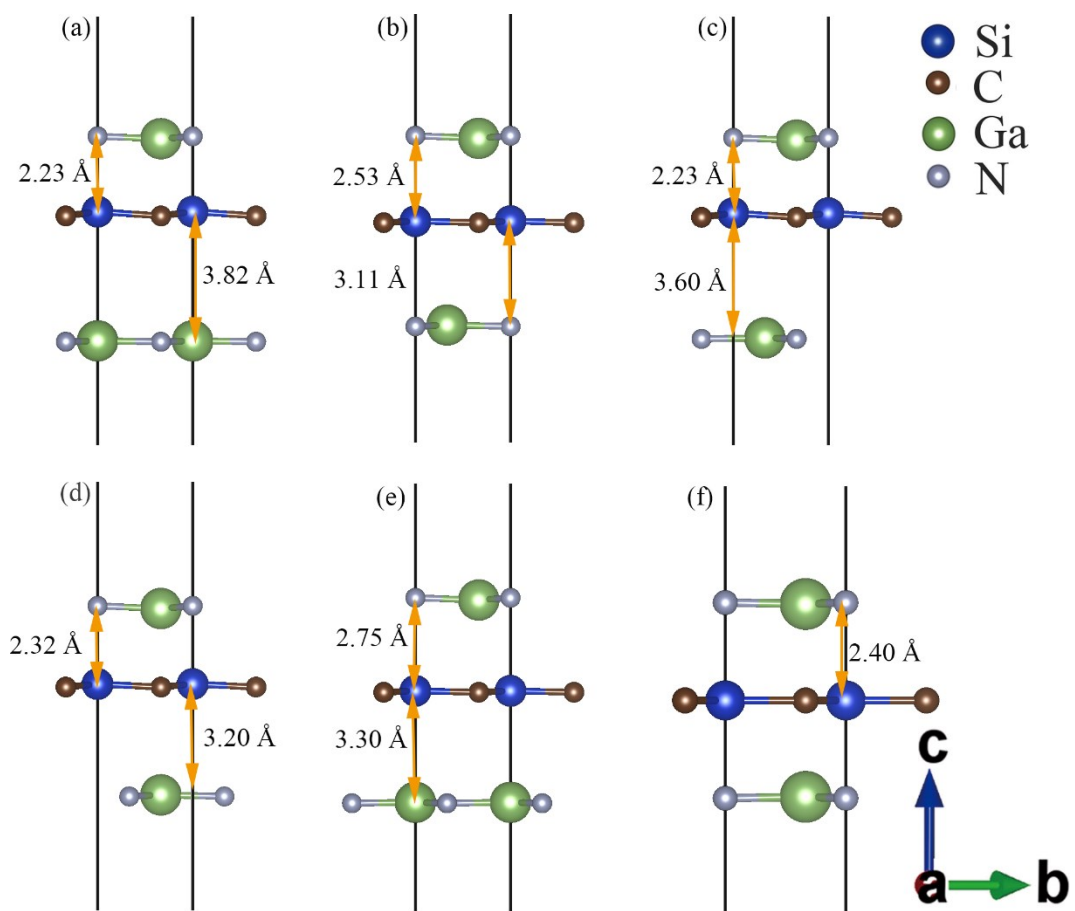


Fig. S2 Side views of the optimized structures of the GaN/SiC/GaN trilayer with different staking. The interlayer spacing (along the z axis) between the individuals of the heterojunctions are calculated and given.

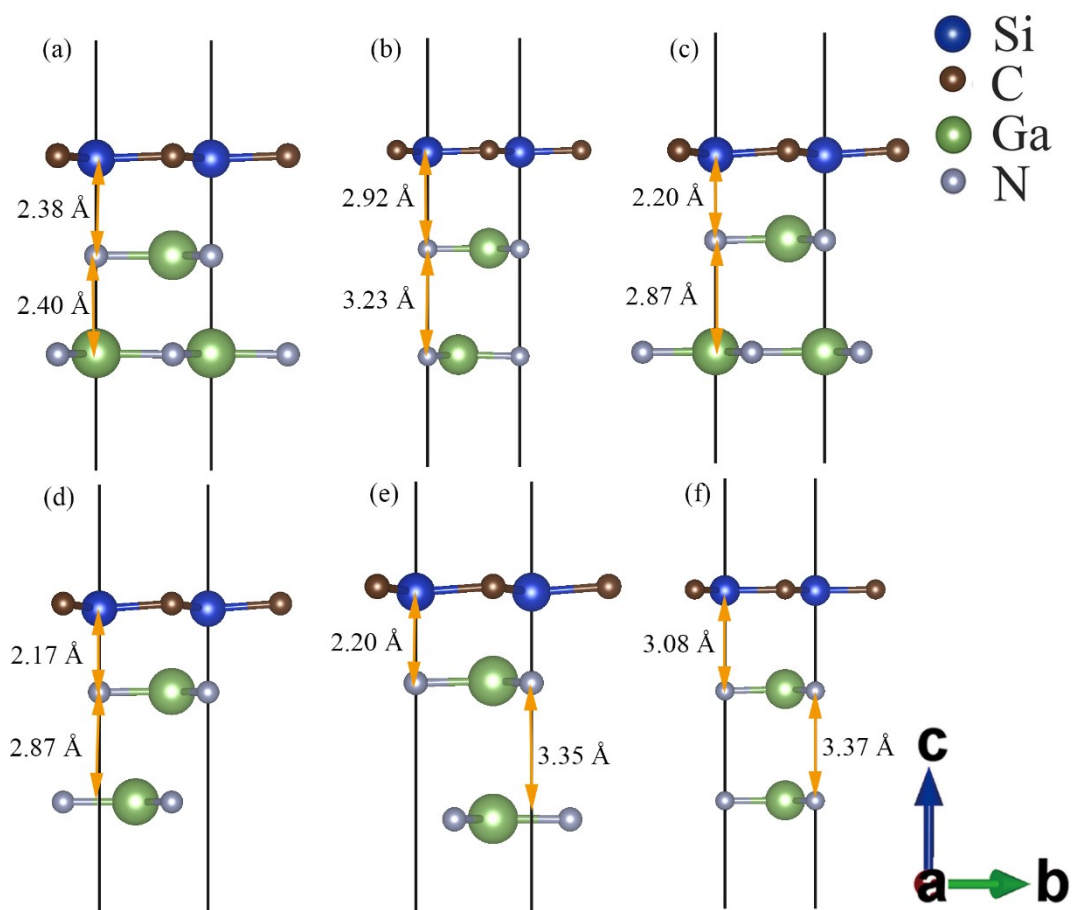


Fig. S3 Side views of the optimized structures of the GaN/GaN/SiC trilayer with different staking. The interlayer spacing (along the z axis) between the individuals of the heterojunctions are calculated and given.

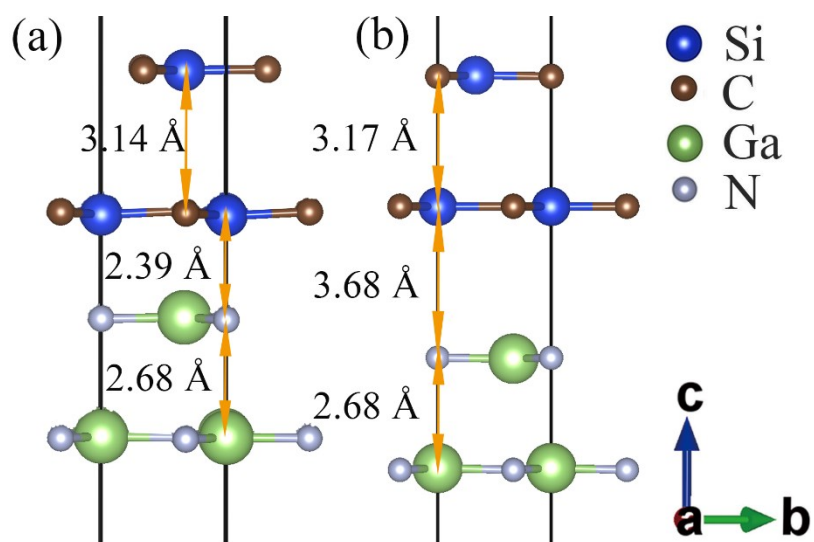


Fig. S4 Side views of the optimized structures of the Bi-GaN/Bi-SiC four layers with different staking. The interlayer spacing (along the z axis) between the individuals of the heterojunctions are calculated and given.

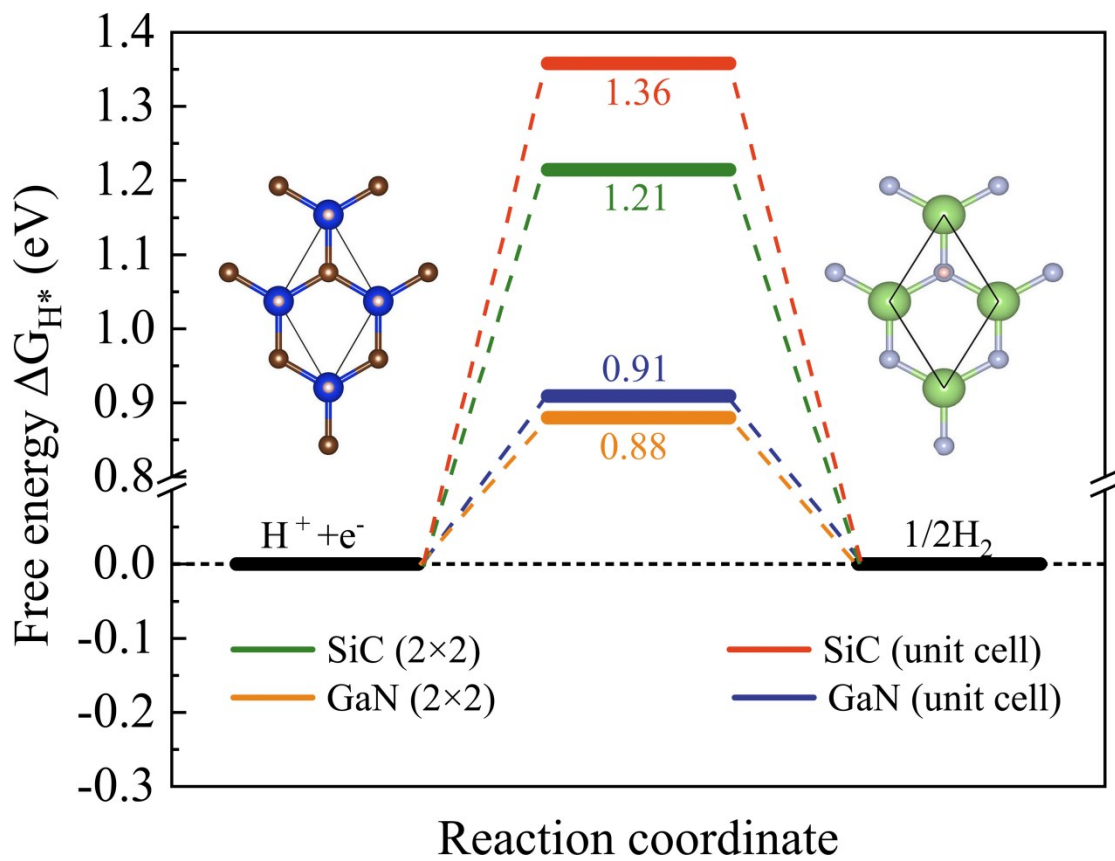


Fig. S5 The calculated free energy diagram of the HER at the equilibrium potential of SiC and GaN monolayers for unit cell and 2×2 supercells.