Support Information for

Two-Dimensional Electron Gas in $MoSi_2N_4/VSi_2N_4$ Heterojunction by First Principles Calculation

Ruiling Gao(高瑞灵) [1†], Chao Liu(刘超) [1†], Le Fang(方乐) [1†*], Bixia Yao(姚碧霞) [1], Wei Wu(吴伟) [1], Qiling Xiao(肖祁陵) [1], Shunbo Hu(胡顺波) [1], Yu Liu(刘禹) [1*], Heng Gao(高恒) [1,2,3,4], Shixun Cao(曹世勋) [1], Guangsheng Song(宋广生) [2], Xiangjian Meng(孟祥建) [4], Xiaoshuang Chen(陈效双) [4], Wei Ren(任伟) [1*]

[1] *Physics Department, State Key Laboratory of Advanced Special Steel, Materials Genome Institute, Shanghai Key Laboratory of High Temperature Superconductors, International Center of Quantum and Molecular Structures, Shanghai University, 200444, Shanghai, China*

[2] *Key Laboratory of Green Fabrication and Surface Technology of Advanced Metal Materials (Anhui University of Technology), Ministry of Education, 243002, Maanshan, China*

[3] *State Key Laboratory of Surface Physics and Department of Physics, Fudan University, 200433, Shanghai, China*

[4] *State Key Laboratory of Infrared Physics, Shanghai Institute of Technical Physics, Chinese Academy of Sciences, 200083, Shanghai, China*

* Corresponding authors: renwei@shu.edu.cn, fangle@shu.edu.cn, ly4209@shu.edu.cn

[†]These authors contributed equally to this work.

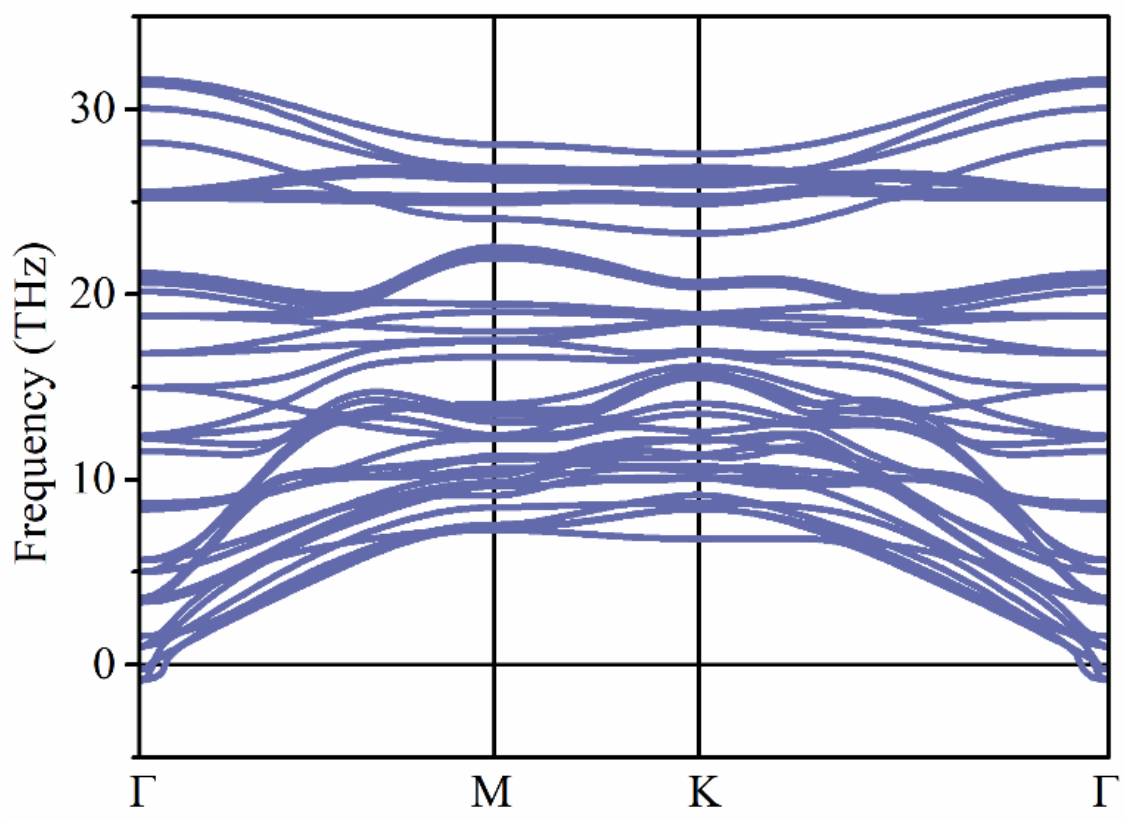

Fig. S1 The calculated phonon dispersion spectra of the most stable AC stacking $MoSi_2N_4/VSi_2N_4$ vertical heterojunction.

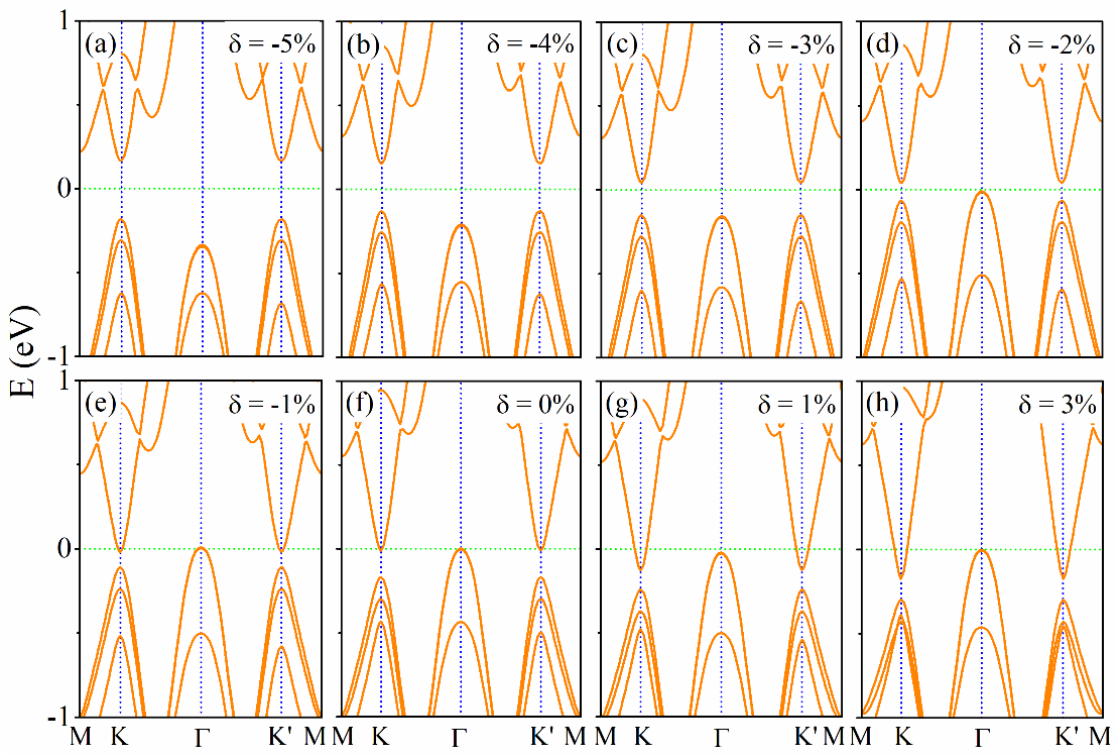

Fig. S2 The band structure of AC heterojunction under different *uniaxial* strain. Panels (a)-(e) are for compressive strain, (f) is unstrained, (g) and (h) are under tensile strain.

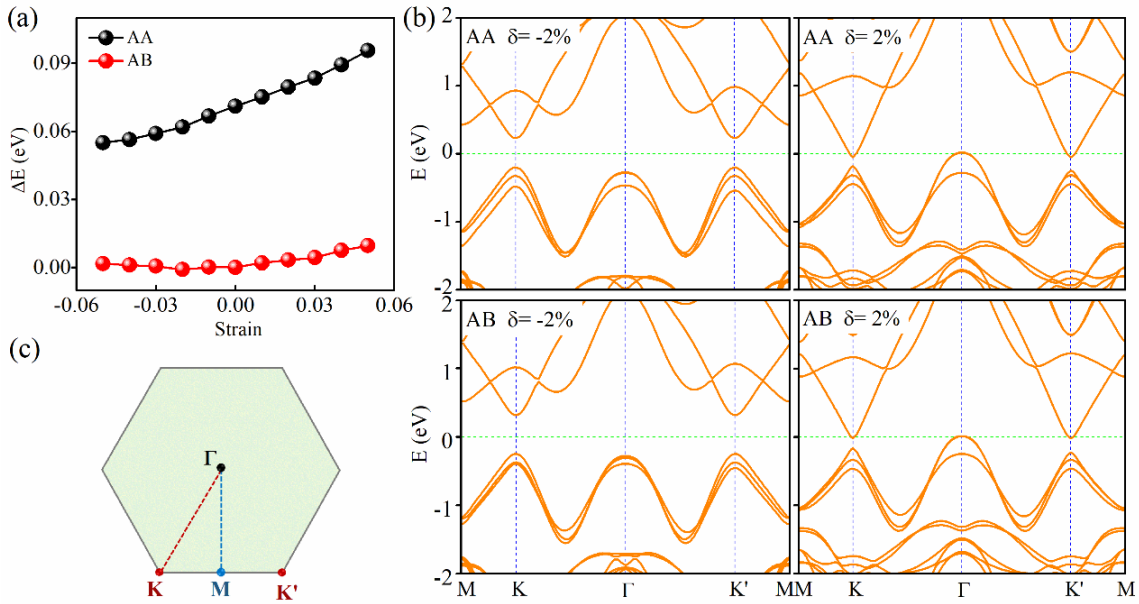

Fig. S3 For the AA and AB heterojunctions under different strain we present in (a) the energy values of AA and AB relative to AC, (b) band structures of AA and AB heterojunctions. Panel (c) shows the first Brillouin zone of the vertical heterojunction systems.

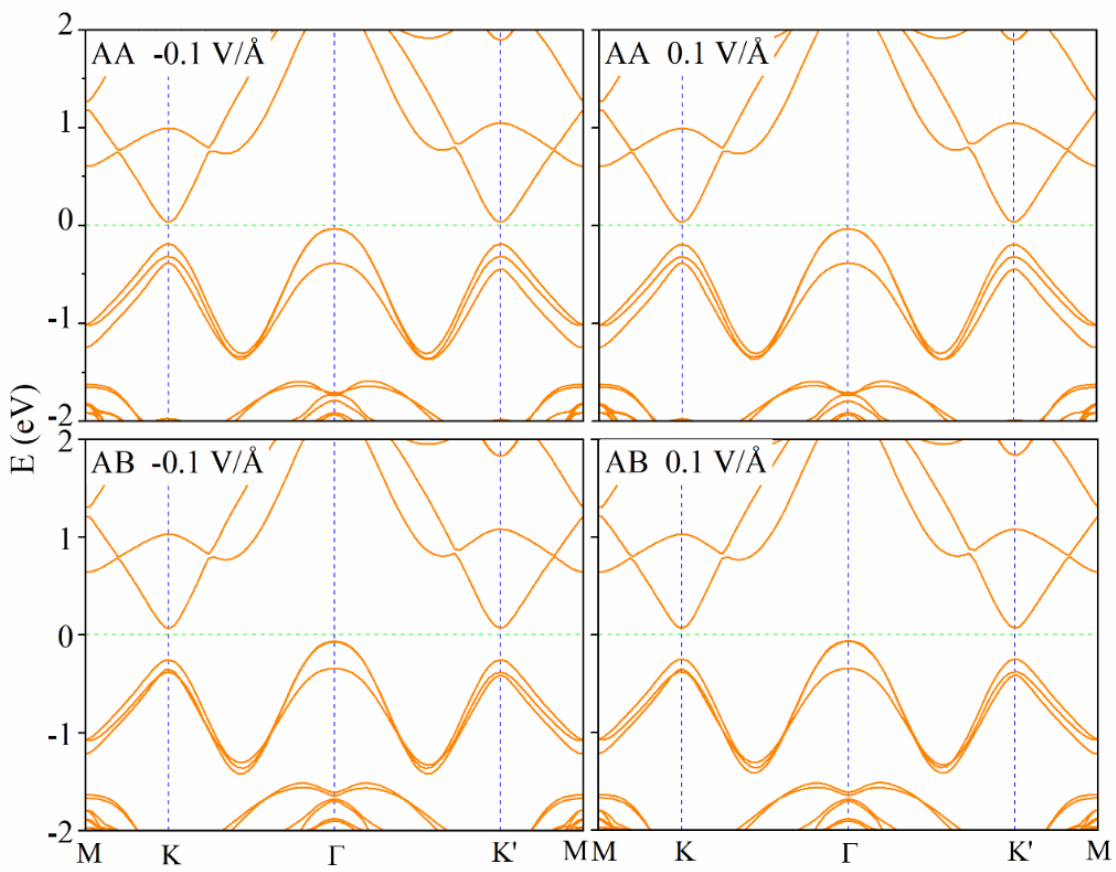

Fig. S4 The band structures of AA and AB heterojunctions under different electric fields.