

**Supplemental Material for  
Robust ferromagnetism in two-dimensional GeC/CrN heterobilayer**

TABLE SI: Structural parameters of the GeC/CrN heterostructure. The lattice constant ( $a$ ), interlayer distance ( $d$ ), buckling parameter ( $\delta_{GeC(CrN)}$ ), binding energy ( $E_b$ ) and charge transfer between CrN and GeC layers ( $\Delta Q$ ), net magnetization ( $M$ ), Hubbard  $U$  parameters.

system	$d$ (Å)	$E_b$ (eV/atom)	$\Delta Q$ ( $ e $ )	$M$ ( $\mu_B$ /per Cr atom)	$U$ (eV)
$\sqrt{7}$ ( $\theta_{TW} = 38.7^\circ$ )	3.13	0.069	0.0665	3.0	4
$\sqrt{13}$ ( $\theta_{TW} = 28.3^\circ$ )	3.14	0.072	0.0564	3.0	4
$\sqrt{19}$ ( $\theta_{TW} = 47.5^\circ$ )	3.05	0.069	0.1034	3.0	4
AA	3.24	0.050	0.0183	3.0	4.2
AB	3.25	0.064	0.0162	3.0	3.8
AA*	2.84	0.099	0.0195	3.0	4.2
AB*	2.79	0.100	0.0646	2.8	3.8

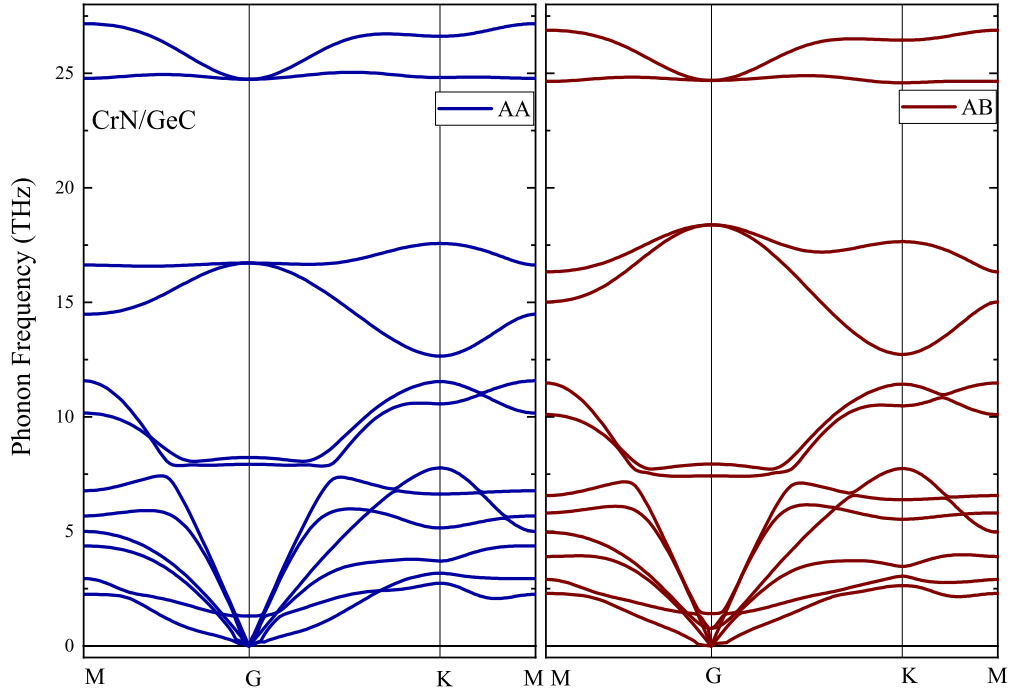


FIG. S1: The phonon spectra of (a) AA and (b) AB stackings of GeC/CrN

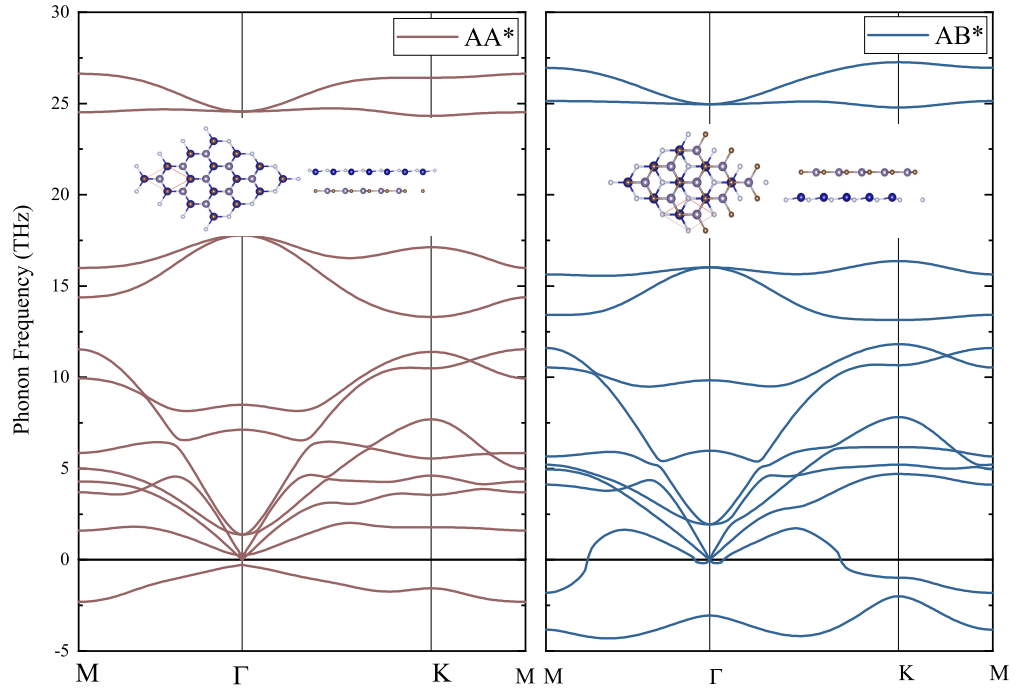


FIG. S2: The phonon spectra of (a) AA\* and (b) AB\* (unstable stackings) of GeC/CrN

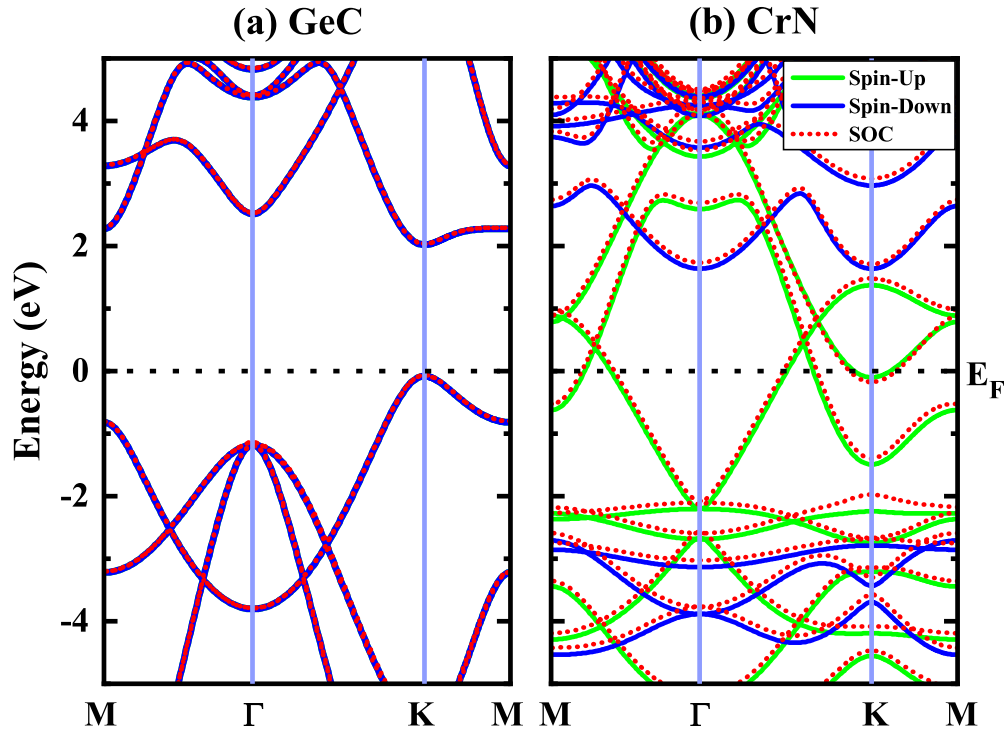


FIG. S3: The energy band spectrum of pristine (a) GeC monolayer and (b) CrN monolayer. The Fermi level is set to be zero.

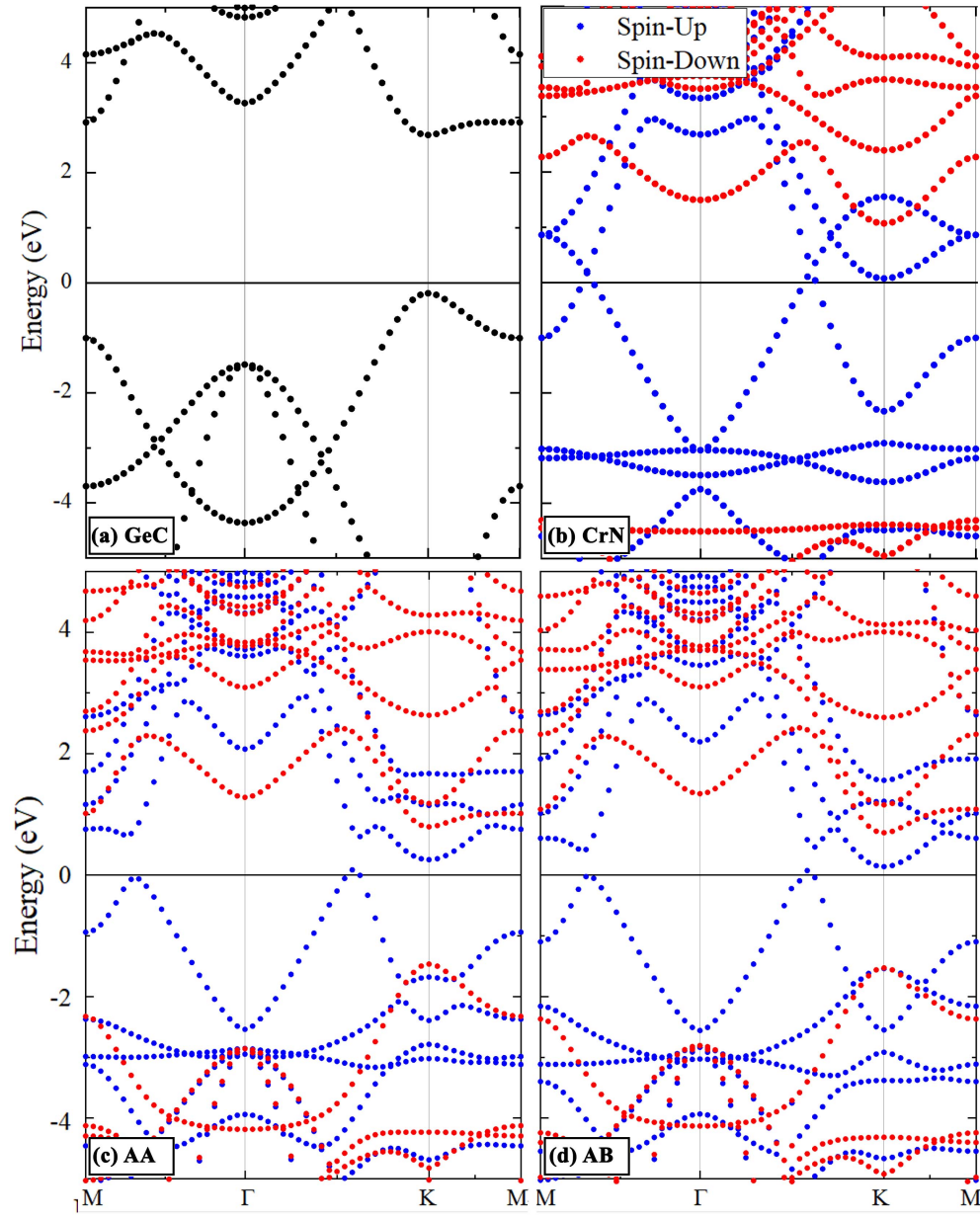


FIG. S4: The energy band spectrum of (a) GeC monolayer and (b) CrN monolayer, (c) AA and (d) AB for HSE06. The Fermi level is set to be zero.

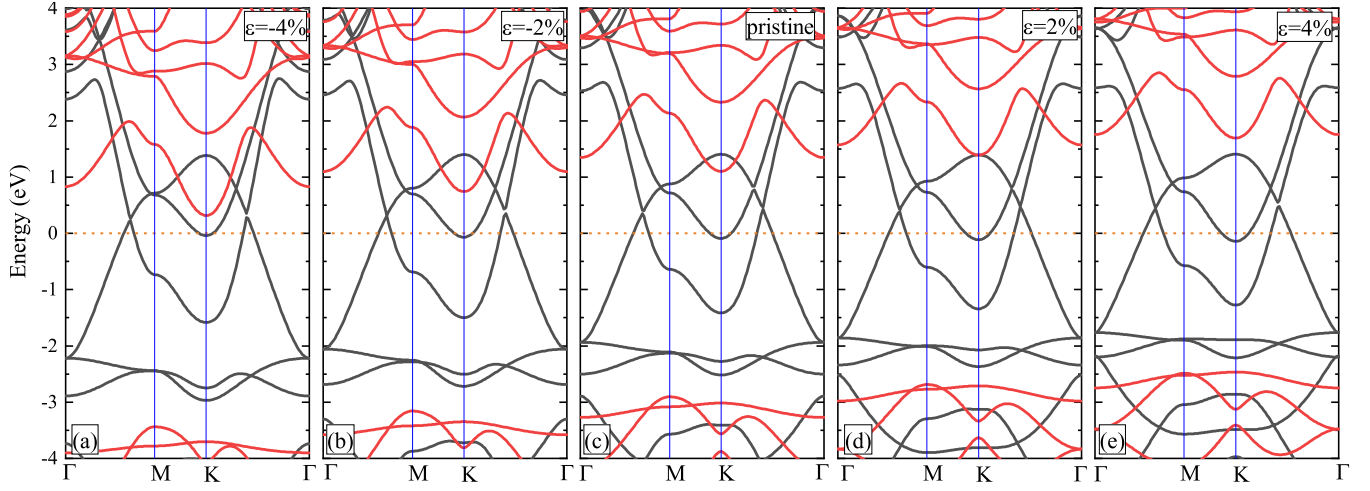


FIG. S5: The band spectrum of monolayer CrN under biaxial strain. The Fermi level is set to be zero.

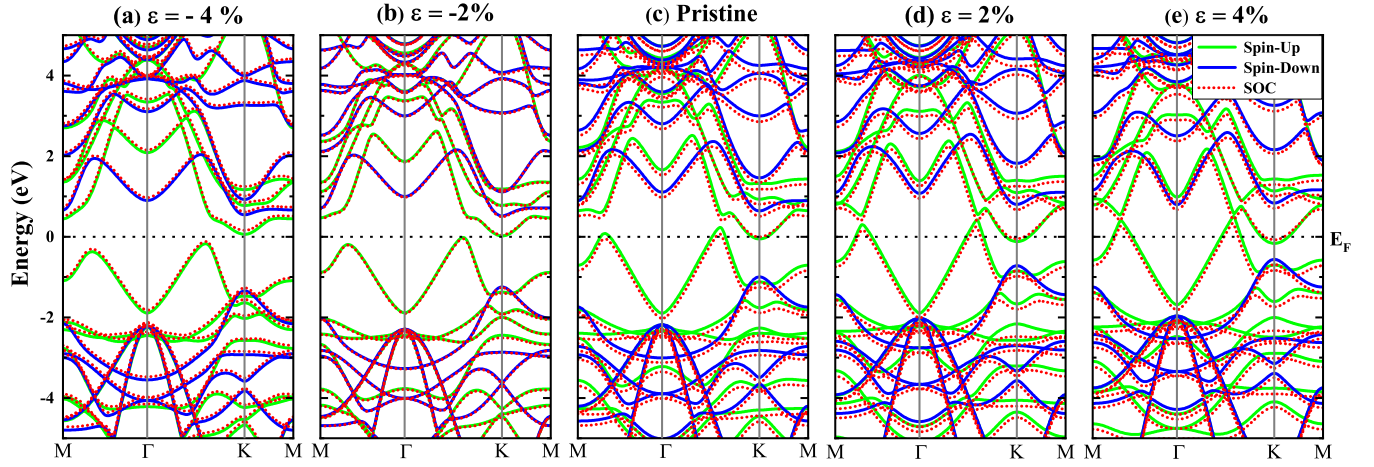


FIG. S6: The band structure of AA for (a)  $\varepsilon = -4\%$ , (b)  $\varepsilon = -2\%$  under compressive strain, (c) pristine, (d)  $\varepsilon = 2\%$ , and (e)  $\varepsilon = 4\%$  under tensile strain. The Fermi level is set to be zero.

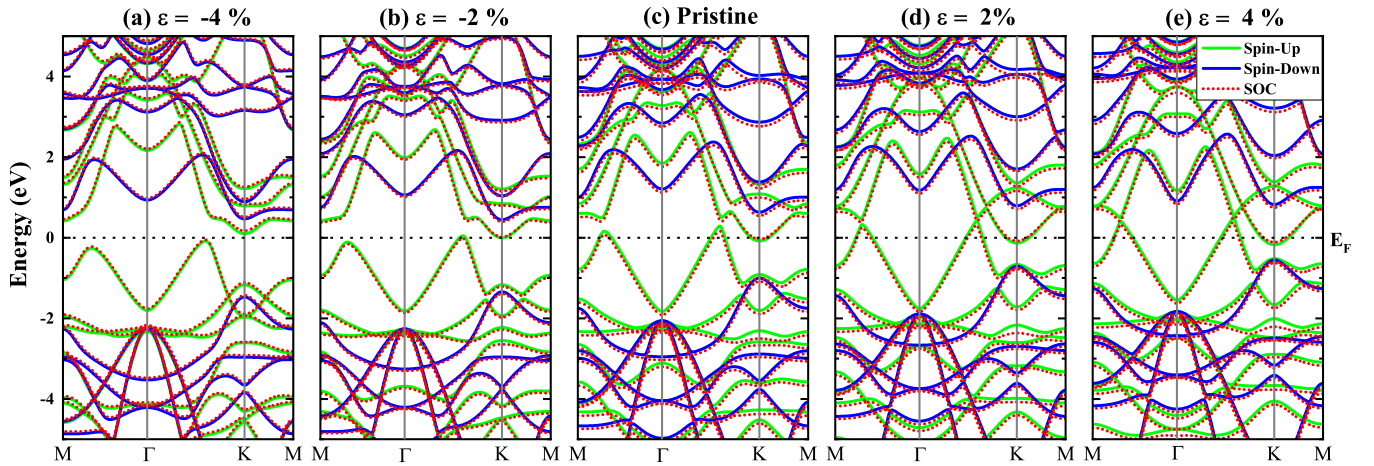


FIG. S7: The band structure of AB for (a)  $\varepsilon = -4\%$ , (b)  $\varepsilon = -2\%$  under compressive strain, (c) pristine, (d)  $\varepsilon = 2\%$ , and (e)  $\varepsilon = 4\%$  under tensile strain. The Fermi level is set to be zero.

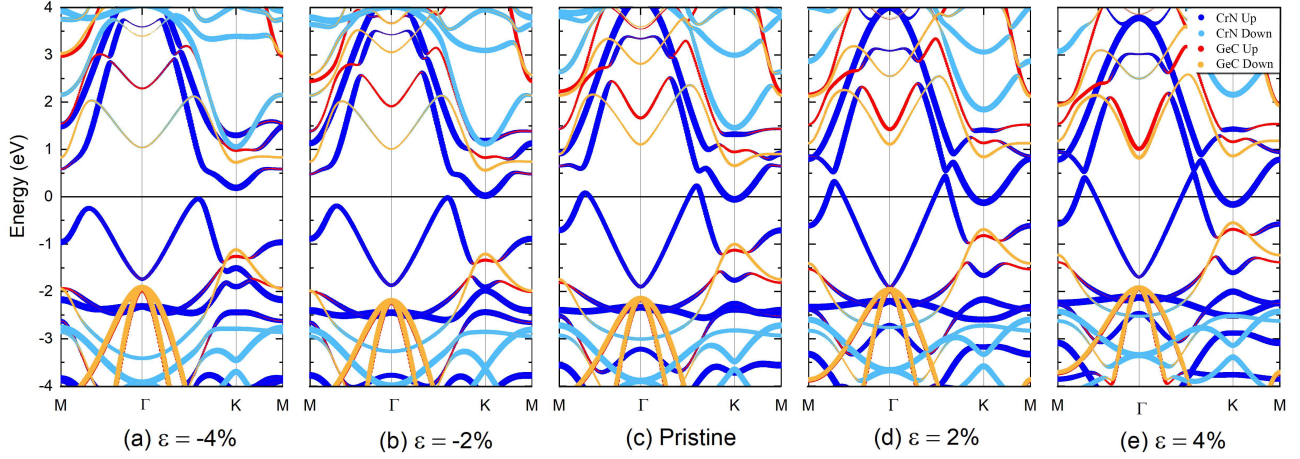


FIG. S8: The partial band structure of AA for (a)  $\varepsilon = -4\%$ , (b)  $\varepsilon = -2\%$  under compressive strain, (c) pristine, (d)  $\varepsilon = 2\%$ , and (e)  $\varepsilon = 4\%$  under tensile strain. The Fermi level is set to be zero.

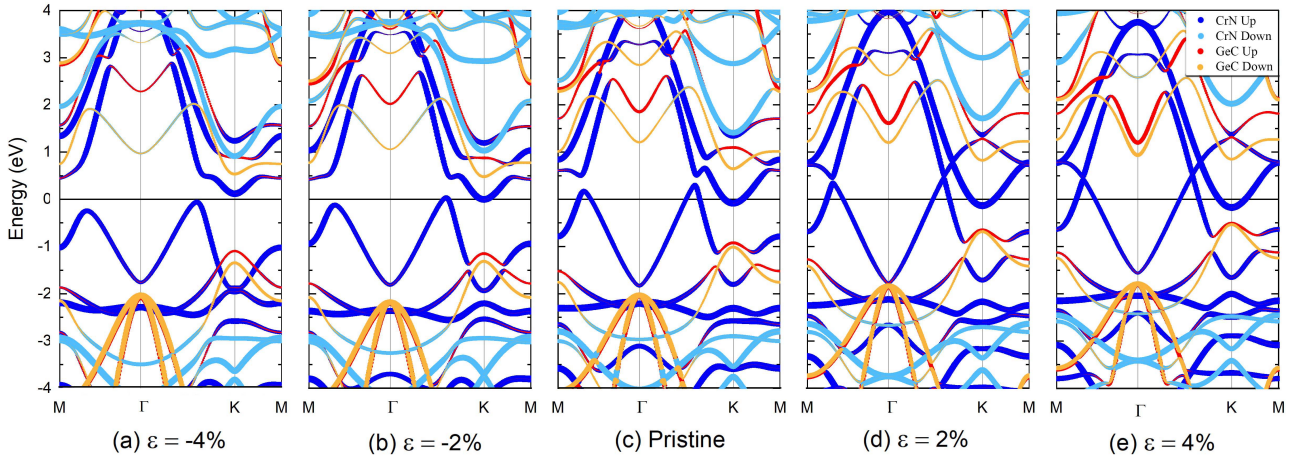


FIG. S9: The partial band structure of AB for (a)  $\varepsilon = -4\%$ , (b)  $\varepsilon = -2\%$  under compressive strain, (c) pristine, (d)  $\varepsilon = 2\%$ , and (e)  $\varepsilon = 4\%$  under tensile strain. The Fermi level is set to be zero.

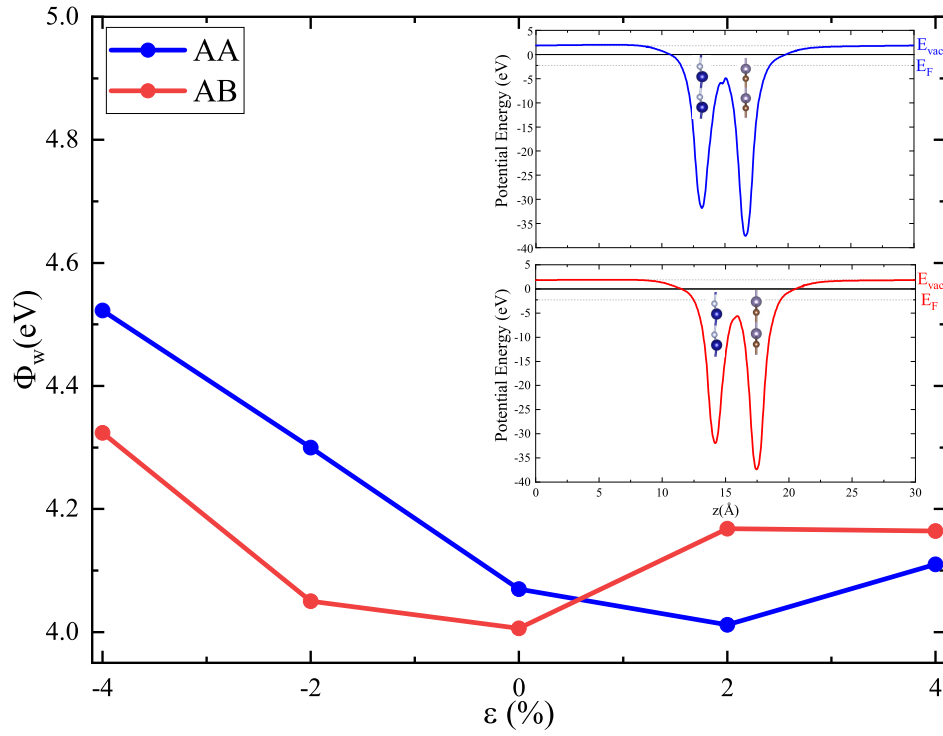


FIG. S10: The calculated work function ( $\Phi_w$ ) of GeC/CrN heterobilayers as a function of strain. Inset: Electrostatic potential energy of AA and AB. The Fermi and the vacuum energies are marked on the potential energy figure.

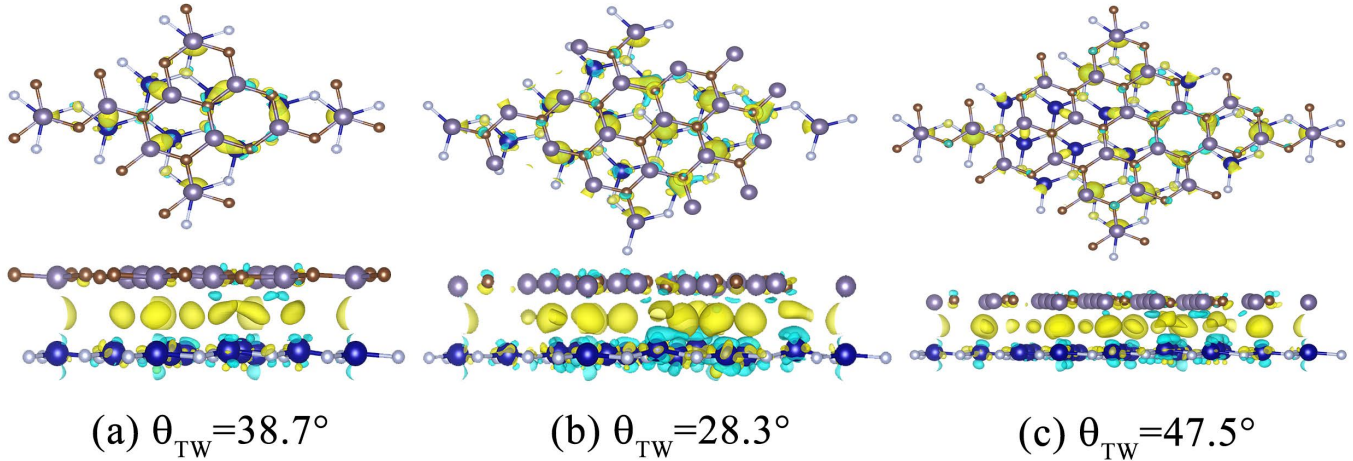


FIG. S11: The charge density differences for (a)  $\theta_{TW} = 38.7^\circ$ , (b)  $\theta_{TW} = 28.3^\circ$  and (c)  $\theta_{TW} = 47.5^\circ$  of twisted GeC/CrN heterobilayer. The isosurface value is set to be  $0.0015 \text{ e}\text{\AA}^{-3}$  for all figures.

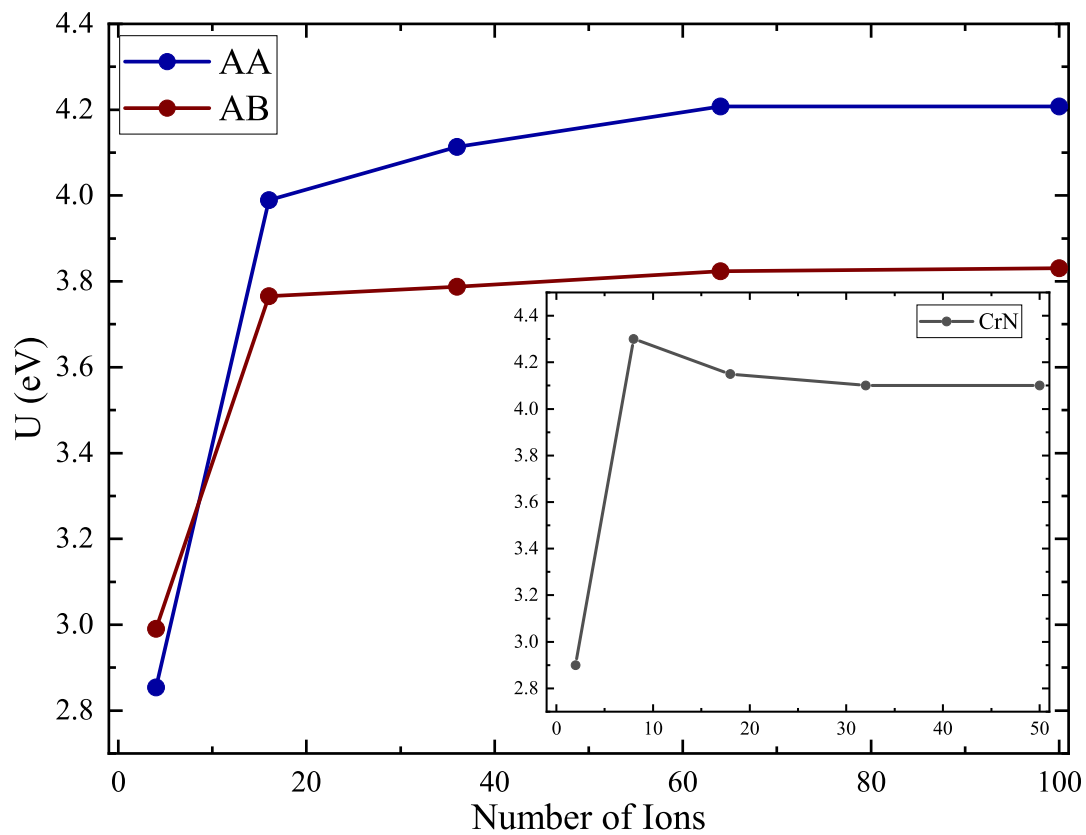


FIG. S12: The calculated Hubbard ( $U$ ) parameters of AA, AB, and CrN monolayer by using the linear response theory.