Supplementary Information

Latent Order in High-Angle Grain Boundary of GaN

Sangmoon Yoon,[1,2] Hyobin Yoo,[1] Seoung-Hun Kang,[2,3] Miyoung Kim,[1,*] and Young-Kyun Kwon[2,3,†]

[1] *Department of Materials Science and Engineering, Seoul National University, Seoul, 08826, Korea*

[2] *Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, Seoul, 02447, Korea*

[3] *Korea Institute for Advanced Study (KIAS), Seoul, 02455, Korea*

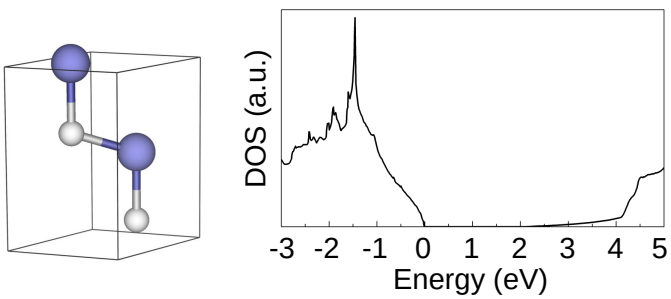

FIG. S1. Atomic structure and DOS of bulk GaN. The band gap of GaN was 2.0eV based on our calculation. The underestimation of band gap is the well-known issue of the LDA calculations.

---

* Corresponding author. E-mail: mkim@snu.ac.kr

† Corresponding author. E-mail: ykkwon@khu.ac.kr

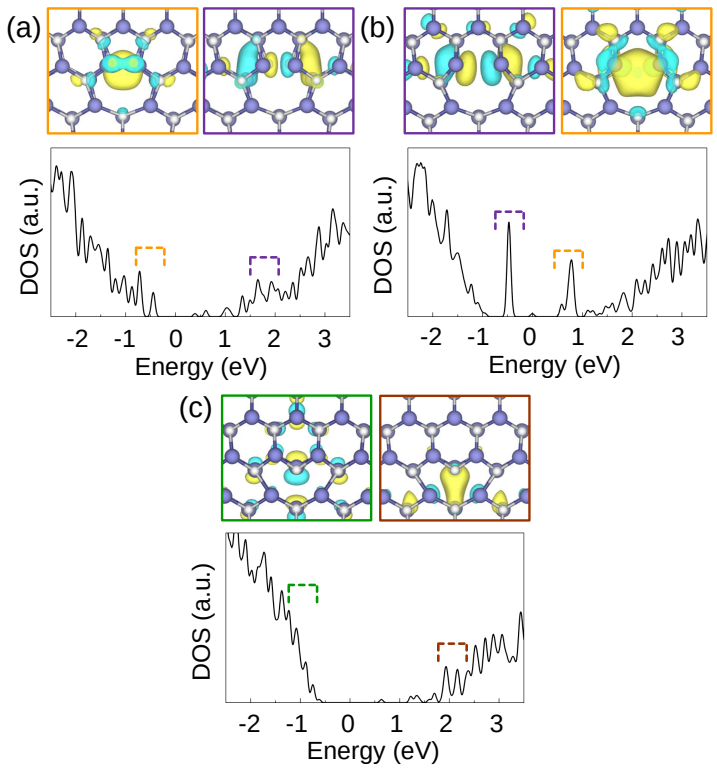

FIG. S2. Wave functions corresponding to defect states localized at the cores of edge dislocations (EDs) and DOS of them: (a) 5/7(S) atom core, (b) 5/7(M) atom core, and (c) 8 atom core. Each wave function enclosed by a specific-colored box was plotted from a defect state bracketed with the same-colored dashed line in the corresponding DOS graph. The localized states of EDs can be directly matched with those of $\Sigma = 7$ CSL boundaries in Fig. 3. However, the energy level of defect states are slightly shifted. For example, the mid-gap states of 5/7 atom cores are relatively shallow in the EDs than in the $\Sigma = 7$ CSL boundaries.