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SUPPLEMENTAL MATERIAL

Si Doping at GaN Inversion Domain Boundaries: an Interfacial Polar Field for Electrons and Holes Separation

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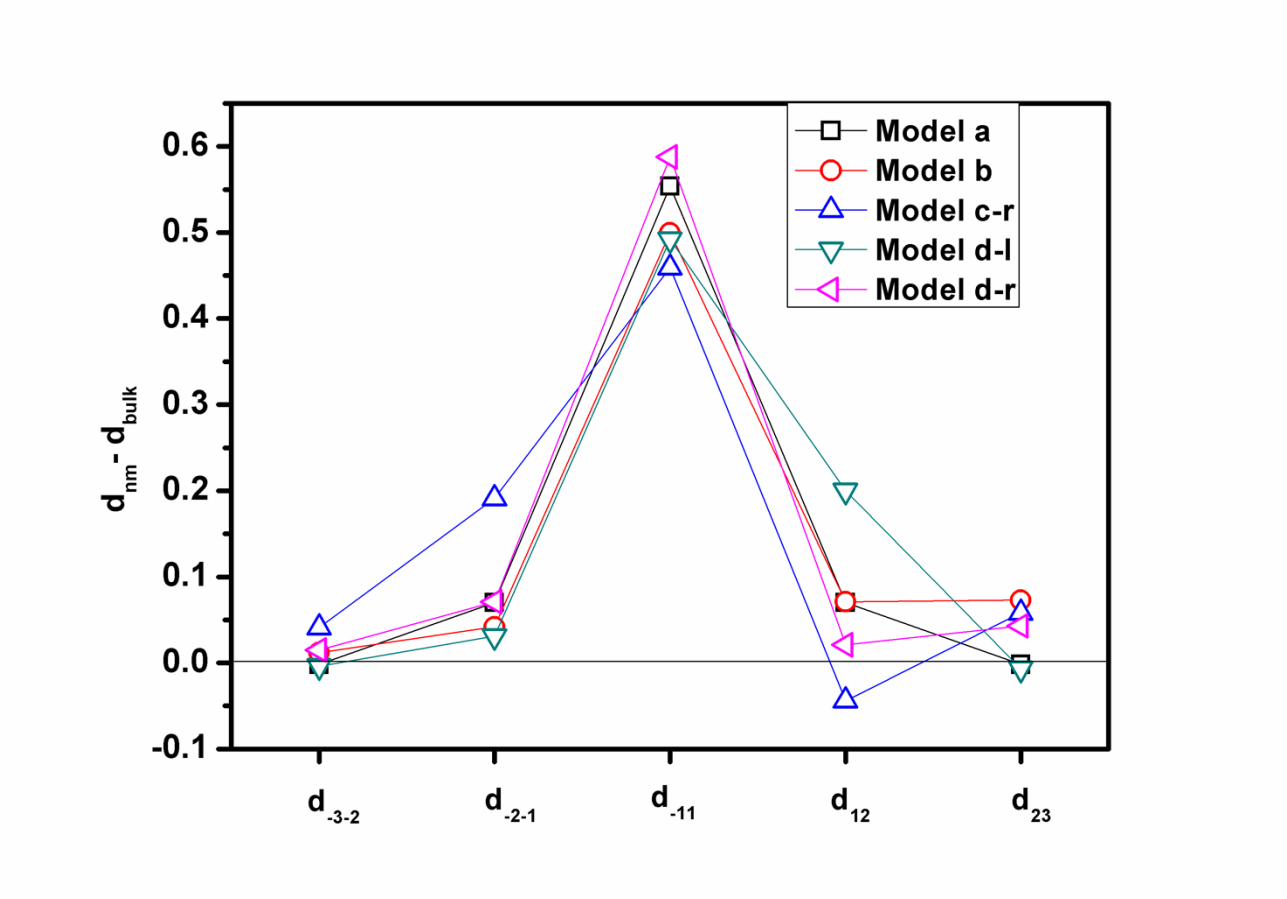

Fig. S1. The interfacial two double layers distances were calculated using the bulk GaN inter- and intra-atomic layer distances as a reference. For bulk GaN, the distance of inter-layer distance is 1.96 Å and the intra-layer distance is 0.96 Å. The suffix –r and –l represent the atoms at the left and right two columns, respectively. The n and m are the layer numbers as show in the right side of Fig. 1.

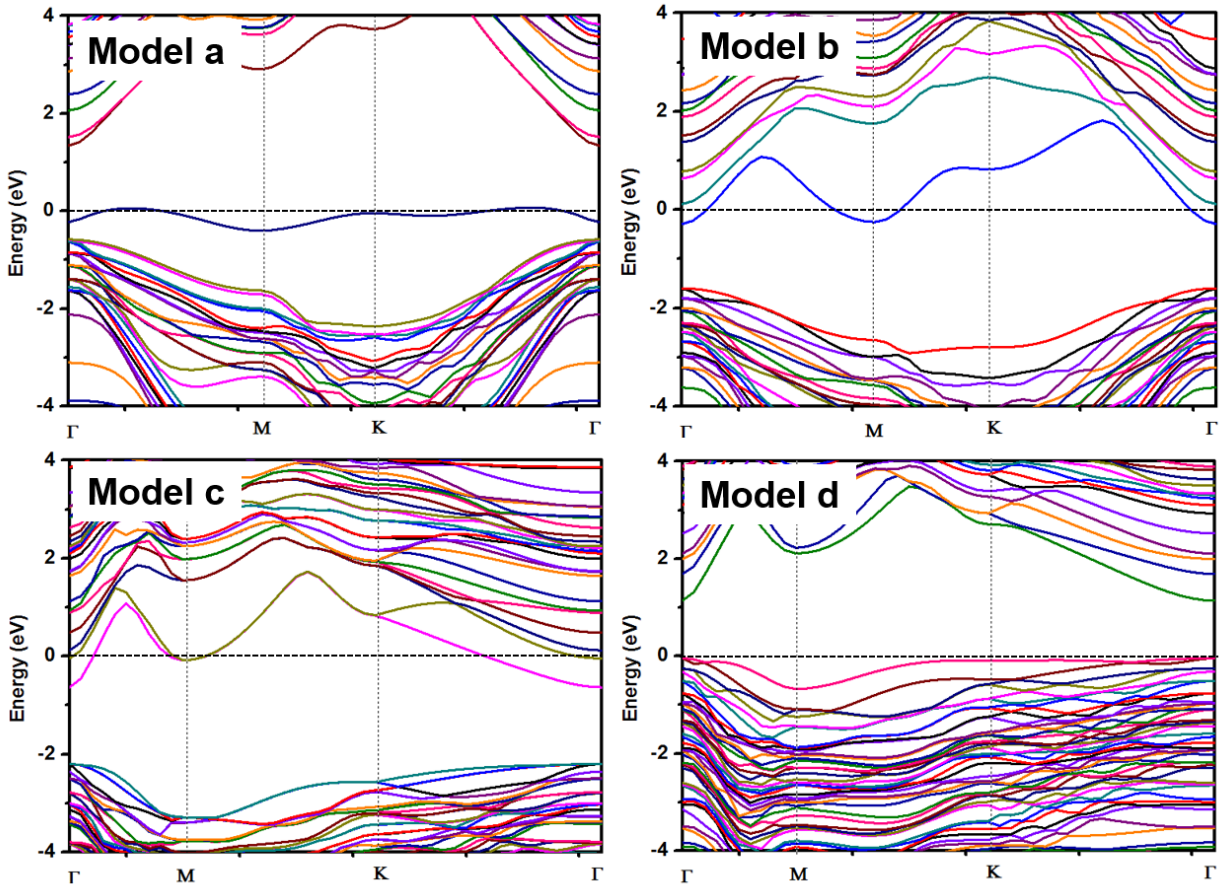

Fig. S2. Band structures of four types of models, and the Fermi level are shown by the dot line. Model (a) exhibits a p-type semiconductor property and Model (b) and (c) have an n-type semiconductor property, while Model (d) characterizes an intrinsic semiconductor.

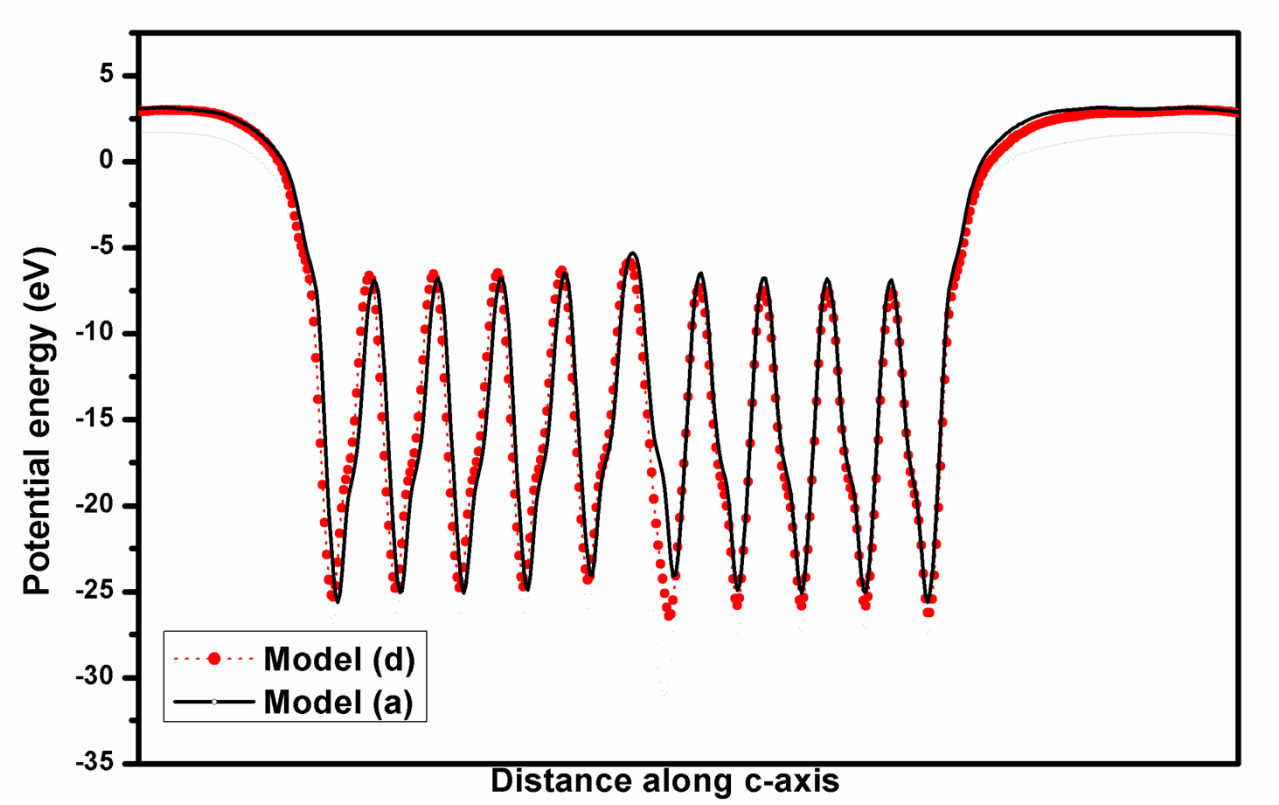

Fig. S3. Plane averaged electron potential energy of model (a) and model (d). For comparison purposes, the Fermi level were aligned to zero. The boundary center have the higher electron potential energy. From model (d), it shows that a potential step of 0.8eV is induced by the local polarity at the right side of the boundary.

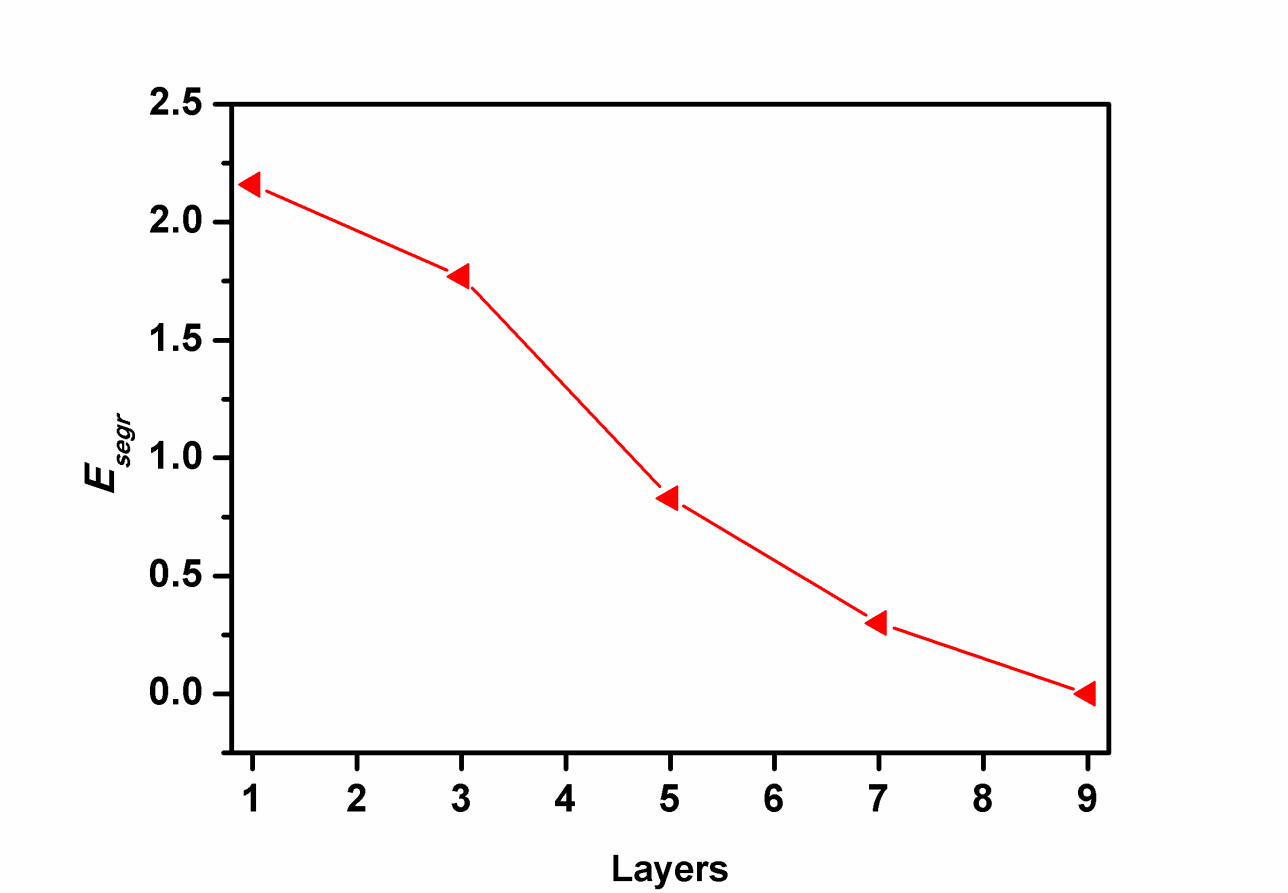

Fig. S4. The segregation energies E_{segr} of the half-monolayer substitution Ga for Si in the depth profile.