SUPPORTING INFORMATION: Onset of vertical bonds in new GaN multilayers: Beyond van der Waals solids

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Figure 1: Phonon spectrum of bilayer structures calculated for $4 \times 4 \times 1$ super cell (256 atoms) (a) Haeckelite-like bilayer; B-HK, new allotropes revealed in this study; (b) B-N1 and (c) B-N2



Figure 2: Perspective views from both sides of the four allotropes of bilayer GaN are shown: (a) Planar bilayer; B-PL, (b) Haeckelite-like bilayer; B-HK, new allotropes revealed in this study; (c) B-N1 and (d) B-N2. Blue and gray balls stand for Ga and N atoms, respectively. Net atomic charges are also given.



Figure 3: Band decomposed charge densities of the planar bilayer B-PL, haeckelite-like bilayer B-HK, new structures B-N1 and B-N2, respectively from top to bottom. Left: Energy bands are displayed along Γ -X direction. Right: Isosurfaces of the charge density distributions of the regarding four conduction and valence band states at the extreme points in Brillouin Zone.



Figure 4: Partial density of states analysis (PDOS) of Planar bilayer; B-PL, Haeckelite-like bilayer; B-HK, new allotropes revealed in this study; B-N1 and B-N2.



Figure 5: Perspective views of the four 3D periodic allotropes of GaN are shown: (a) periodic layered, P-PL, (b) periodic haeckelite-like, P-HK, (c) periodic new structure, P-N2 and (d) wurtzite, WZ. Blue and gray balls stand for Ga and N atoms, respectively. Net atomic charges are also given.



Figure 6: Phonon spectrum of periodic structures (a) periodic haeckelite-like, P-HK, (b) periodic new structure, P-N2 and (c) Brillouin zone.



Figure 7: Band decomposed charge densities of the planar periodic P-PL, haeckelite-like periodic P-HK, periodic new structure, P-N2, and 3D wurtzite WZ structures, respectively from top to bottom. Left: Energy bands are displayed along Γ -X direction. Right: Isosurfaces of the charge density distributions of the regarding four conduction and valence band states at the extreme points in Brillouin Zone.



Figure 8: Partial density of states analysis (PDOS) of the planar periodic P-PL, haeckelitelike periodic P-HK, periodic new structure, P-N2, and 3D wurtzite WZ structures, respectively from top to bottom.