Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material

Theoretical discovery of novel two-dimensional of V^A-N binary compounds with auxiticity

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Figure S1

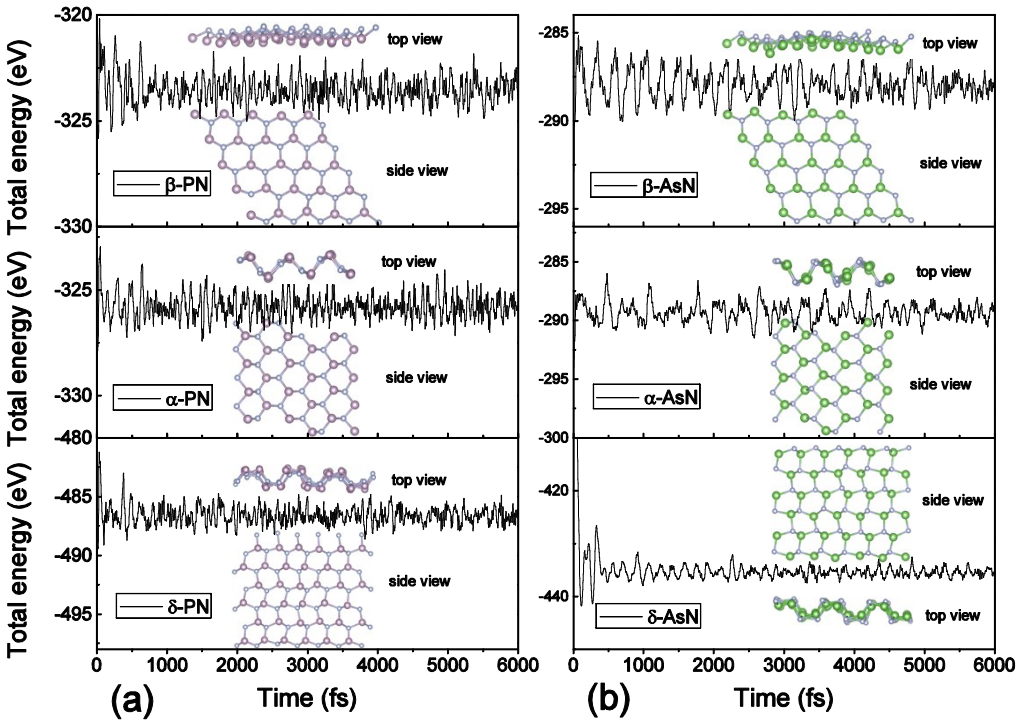

Figure S1. Variations of total energy with respect to time for (a) PN and (b) AsN structures during molecular dynamics simulations at 750 K. Supercell with 50, 48, and 72 atoms is used for structures in β-, α-, and δ-phases, respectively.

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Figure S2

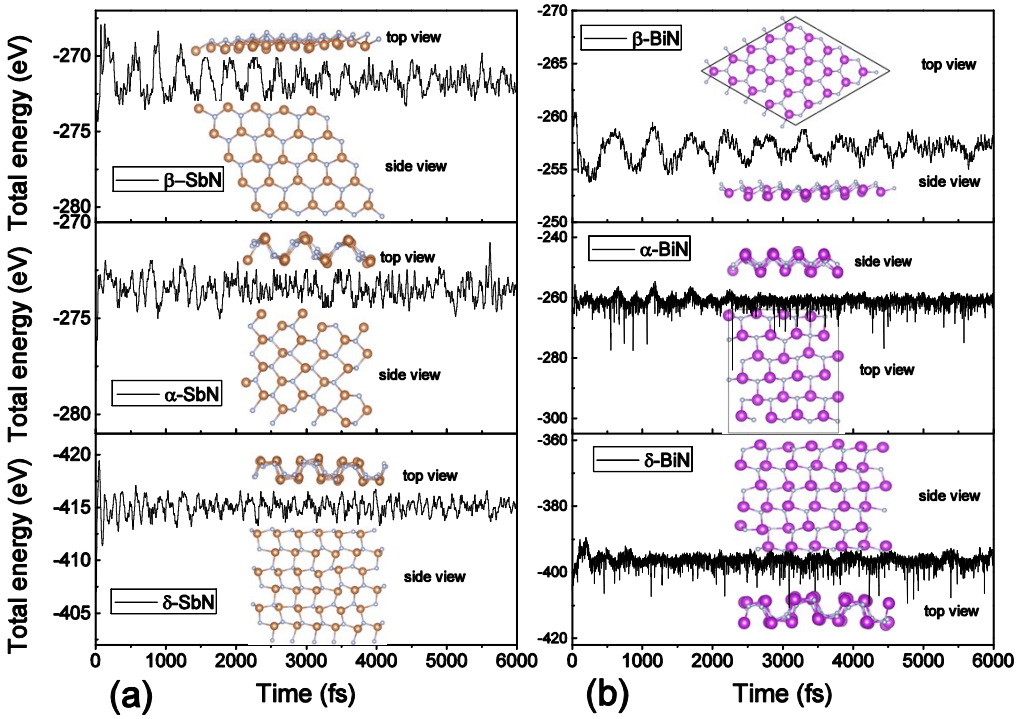

Figure S2. Variations of total energy with respect to time for (a) SbN and (b) BiN structures during molecular dynamics simulations at 750 K. Supercell with 50, 48, and 72 atoms is used for structures in β, α, and δ phases, respectively.

Figure S3:

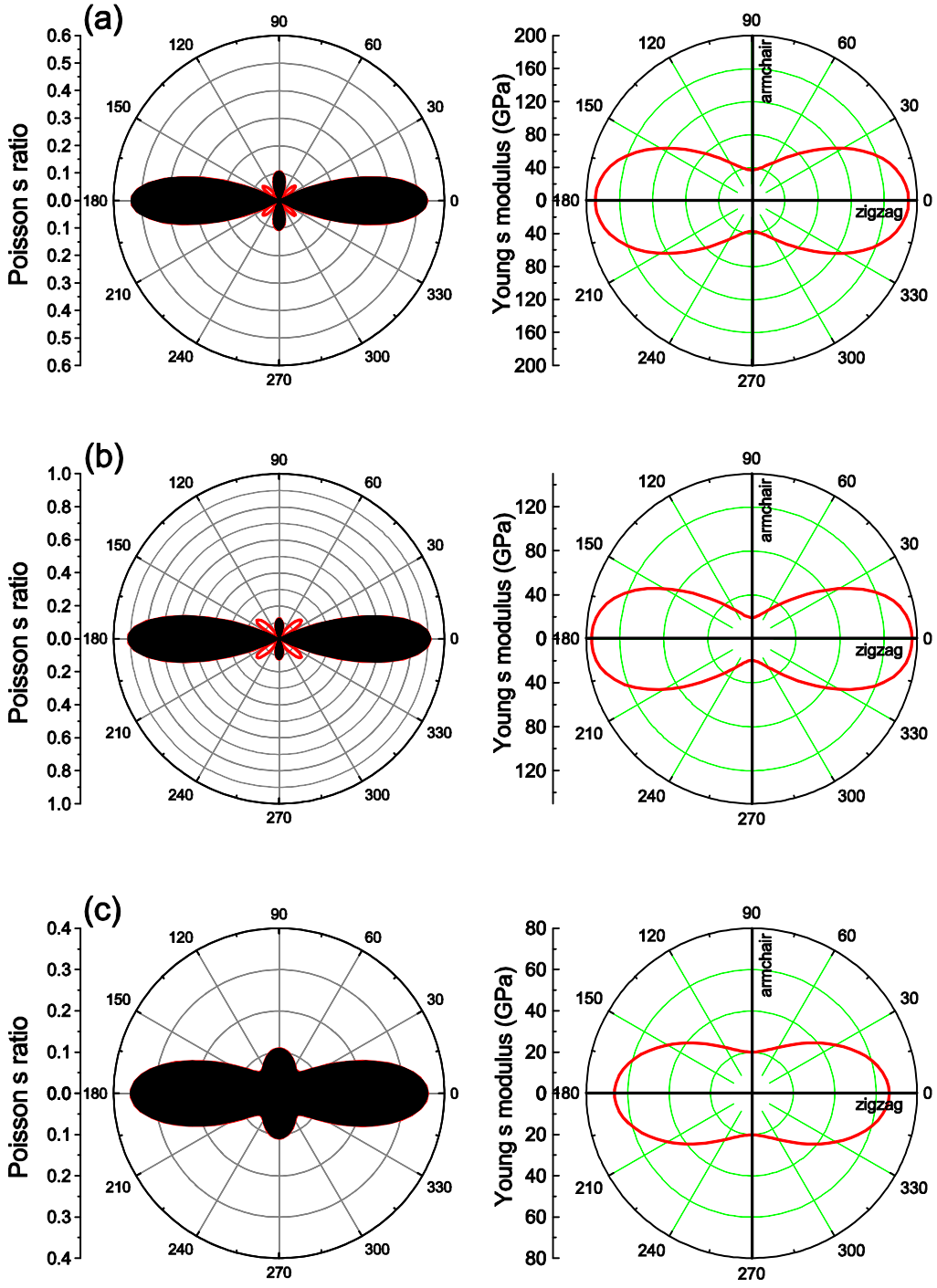

Figure S3. Polar diagram for the Poisson ratio $\nu(\theta)$ and Young's modulus $Y(\theta)$ of (a) δ-NP, (b) δ-AsN and (c) δ-BiN. The angle θ identifies the extension direction with respect to the zigzag (x) direction. The shaded area corresponds to positive Poisson ratio values.

Figure S4:

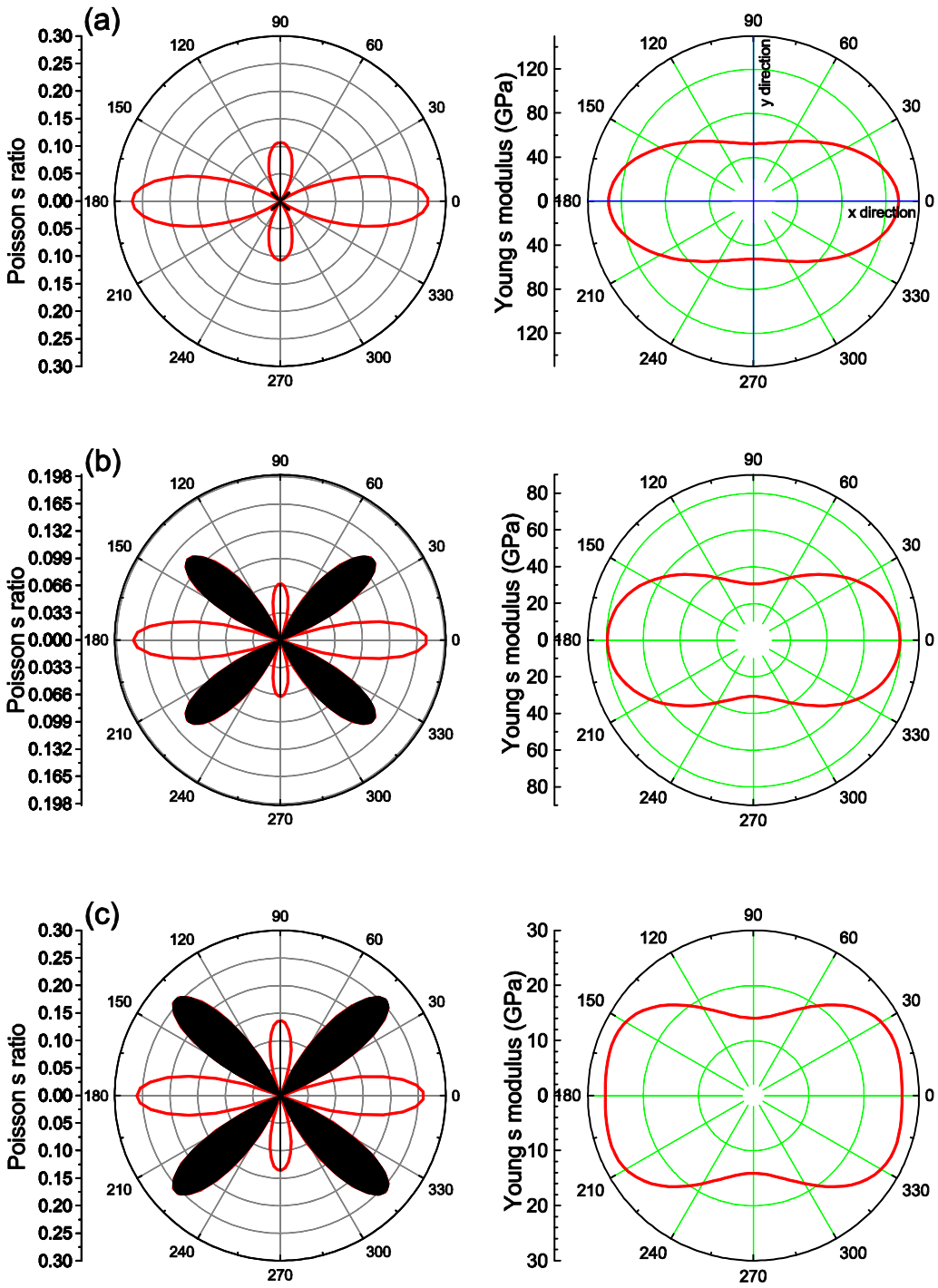

Figure S4. Polar diagram for the Poisson ratio $\nu(\theta)$ and Young's modulus $Y(\theta)$ of (a) α-PN, (b) α-AsN and (c) α-BiN. The angle θ identifies the extension direction with respect to the zigzag (x) direction. The shaded area corresponds to positive Poisson ratio values.

Figure S5:

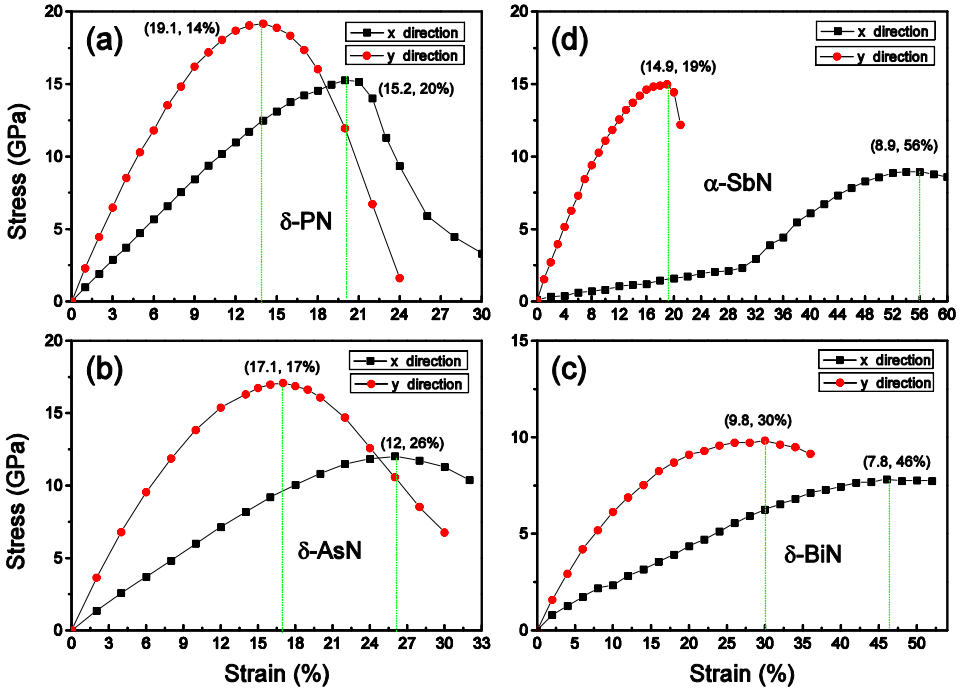

Figure S5. The strain-stress relation for 2D (a) δ-PN (b) δ-AsN, (c) α-SbN, and (d) δ-BiN structure with uniaxial load.

Figure S6:

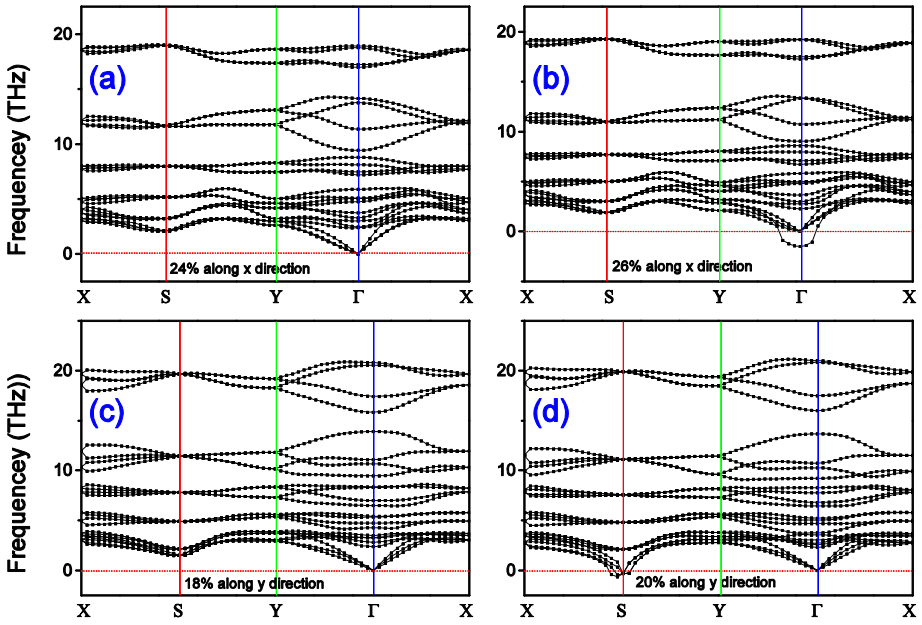

Figure S6. Phonon bands of δ-SbN at different uniaxial strains: (a) 18% and (b) 20% along the *x* direction, and (c) 24% and (d) 26% along the *y* direction.

Figure S7.

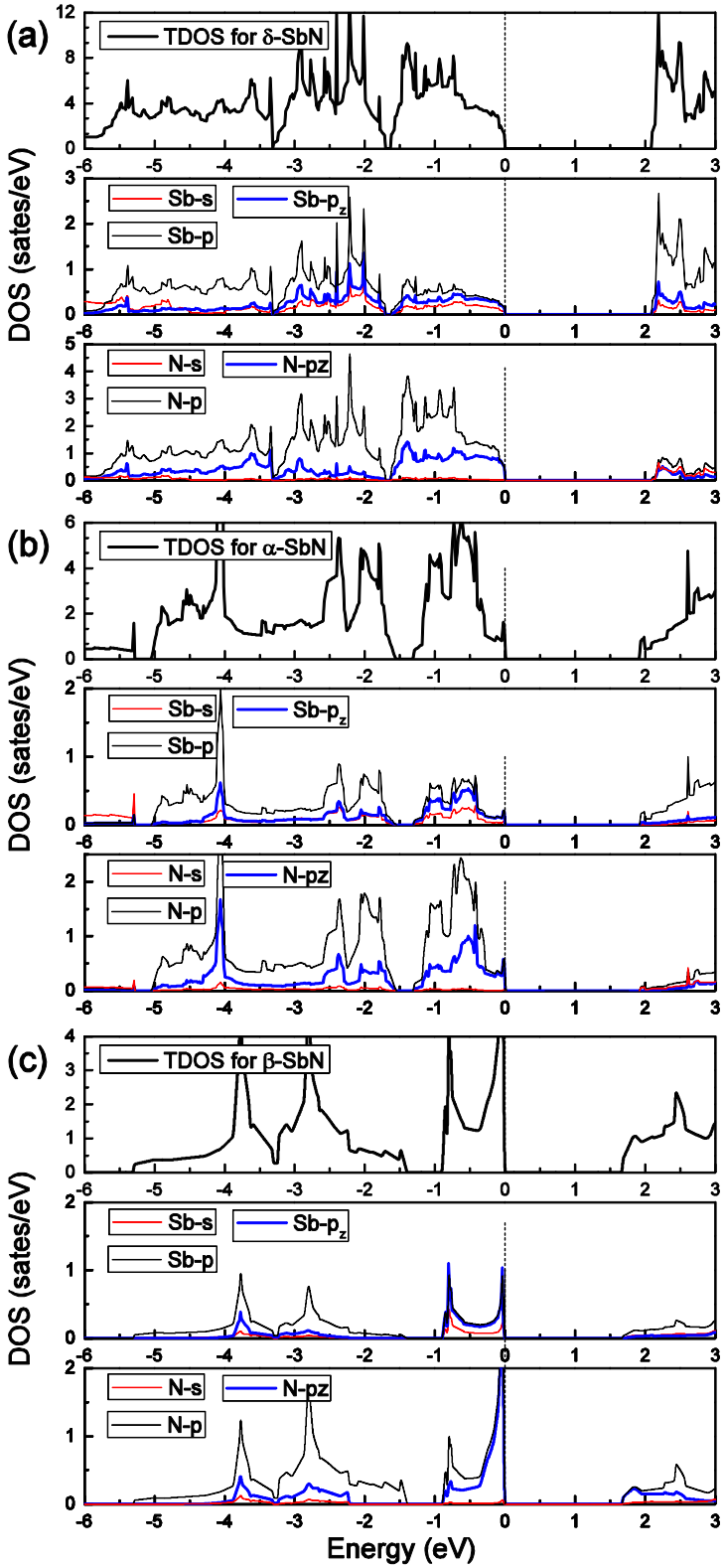

Figure 7. Total and partial DOS of the (a) δ-, (b) α-, and (c) β-SbN monolayer.

Figure 8

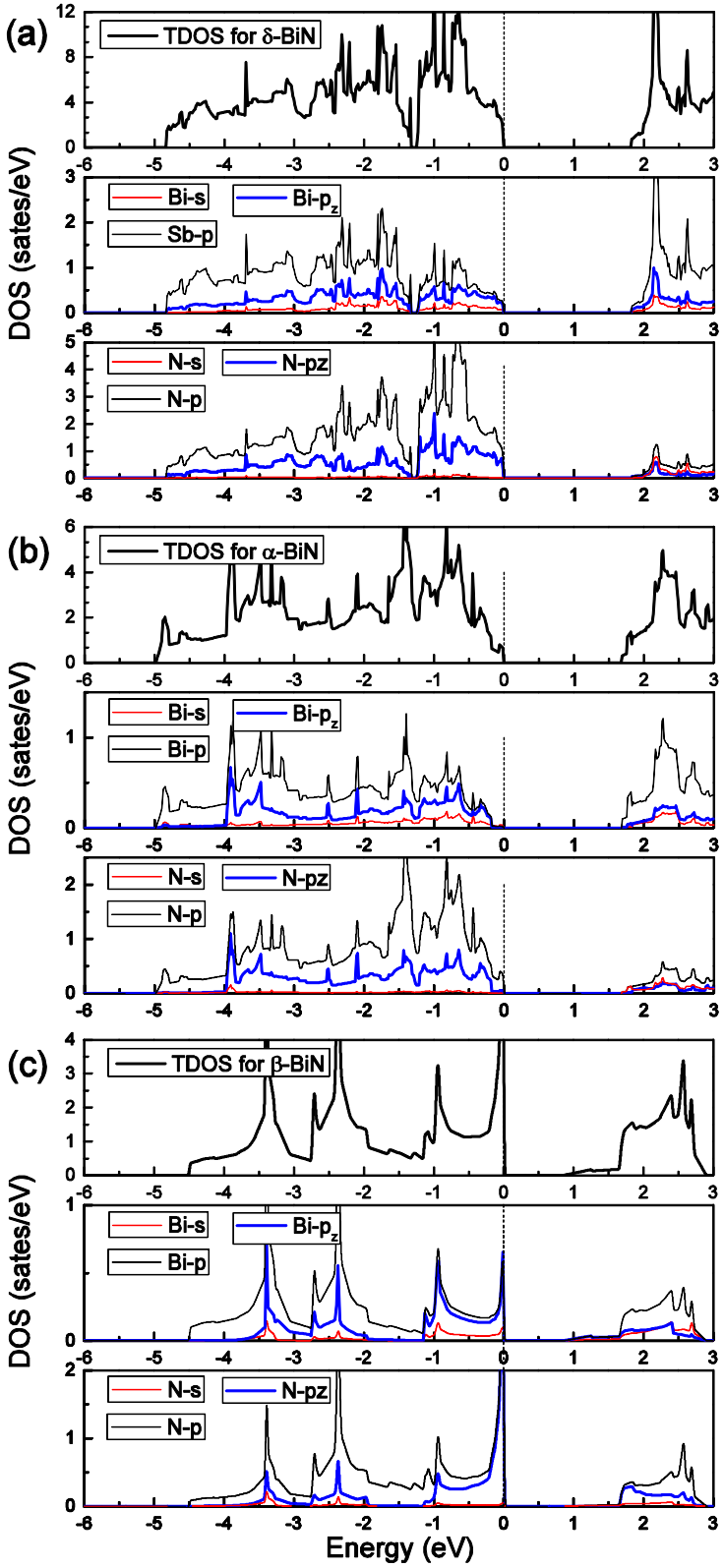

Figure 8. Total and partial DOS of the (a) δ-, (b) α-, and (c) β-BiN monolayer.