# Supporting Information

## Band Gap Opening in Stanene Induced by Patterned B-N doping

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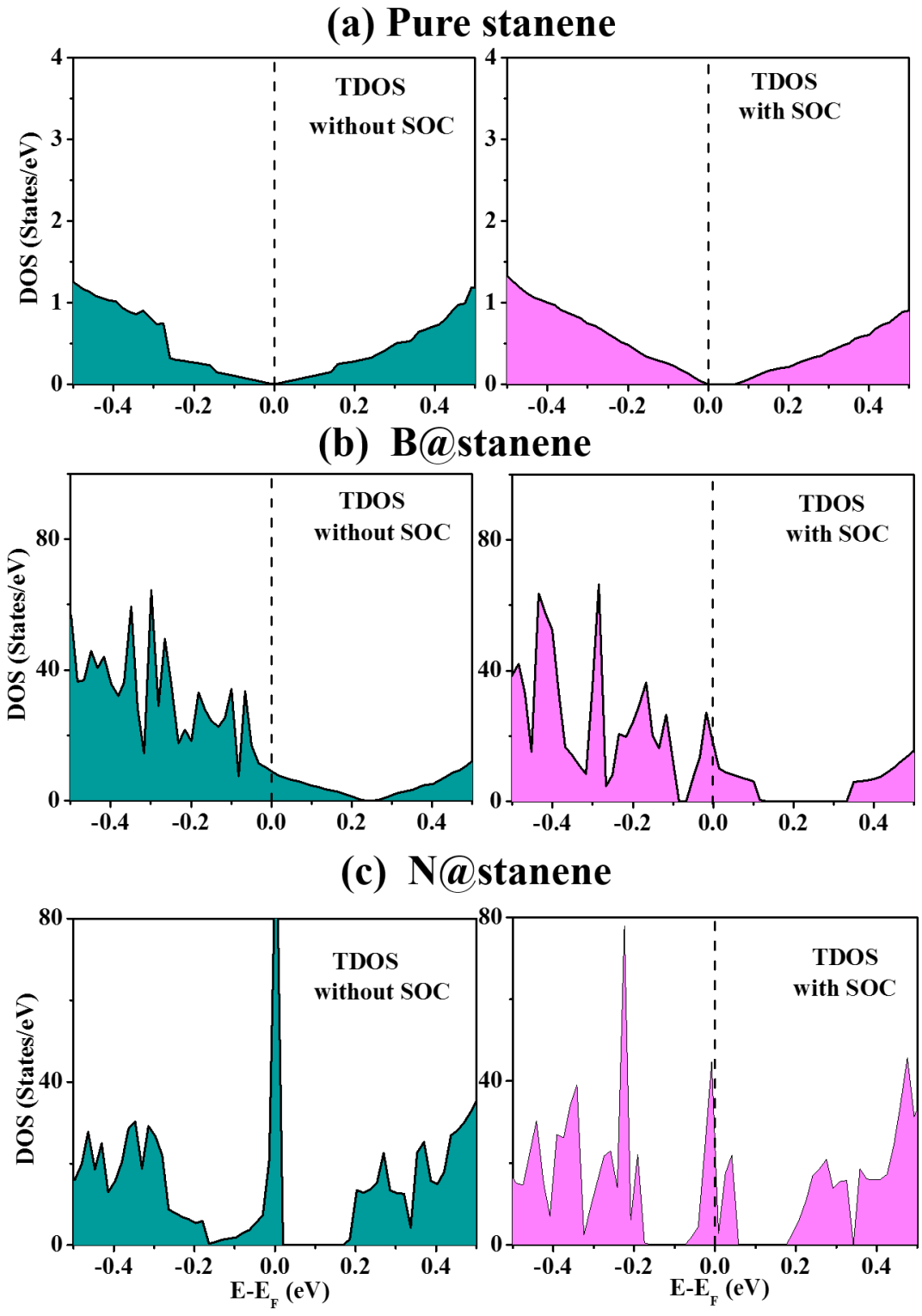


**Figure S1:** Total density of states [with and without the effect of spin orbit coupling (SOC)] of (a) pure stanene, (b) B@stanene, and (c) N@stanene, respectively. The Fermi level shifted to zero, indicated by black dashed line.

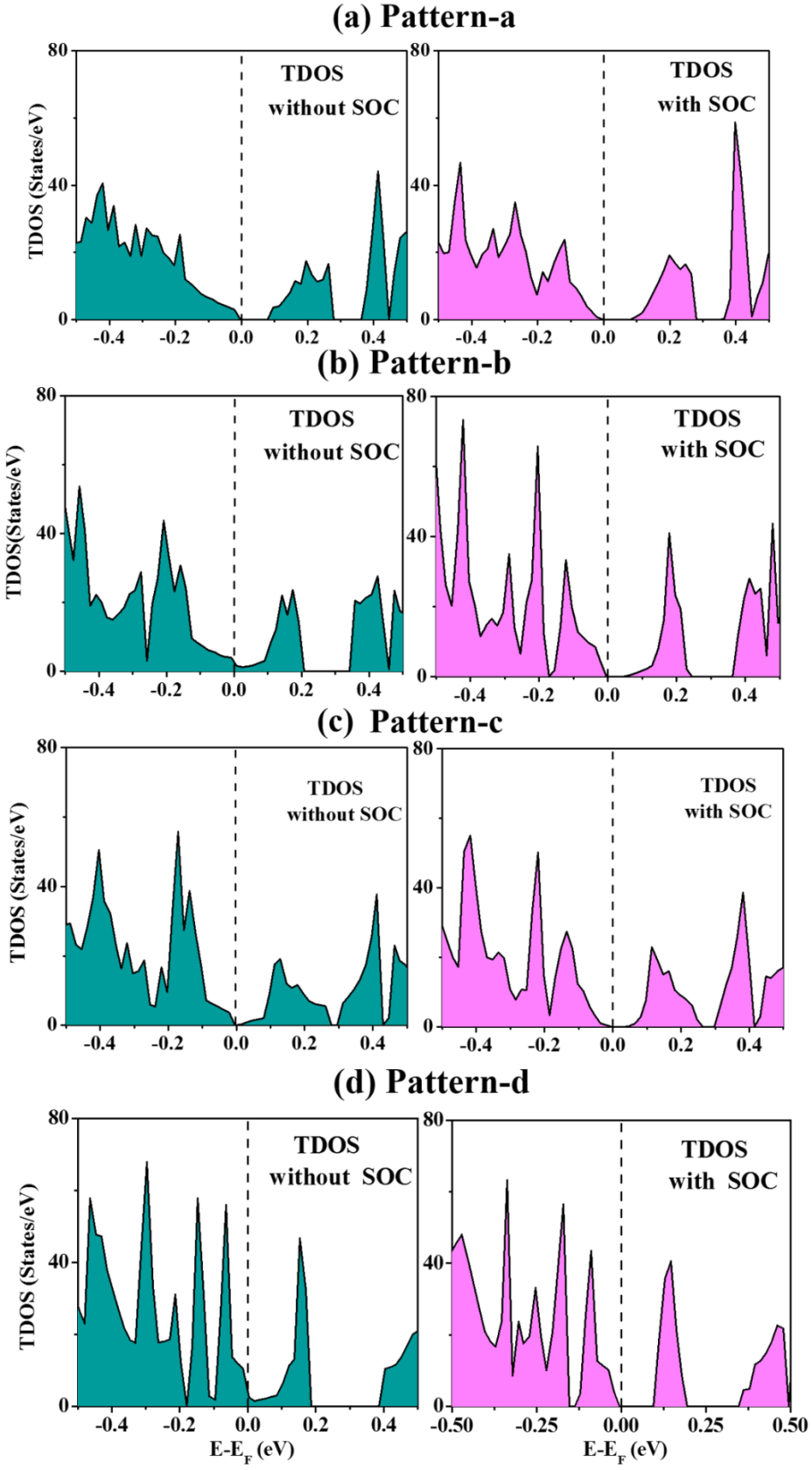


**Figure S2: Figure S2:** Total density of states [with and without the effect of spin orbit coupling (SOC)] of B-N@stanene of (a) pattern-a, (b) pattern-b, (c) pattern-c, and (d) pattern-d, respectively. Fermi level is shifted to zero and indicated by a black dashed line.

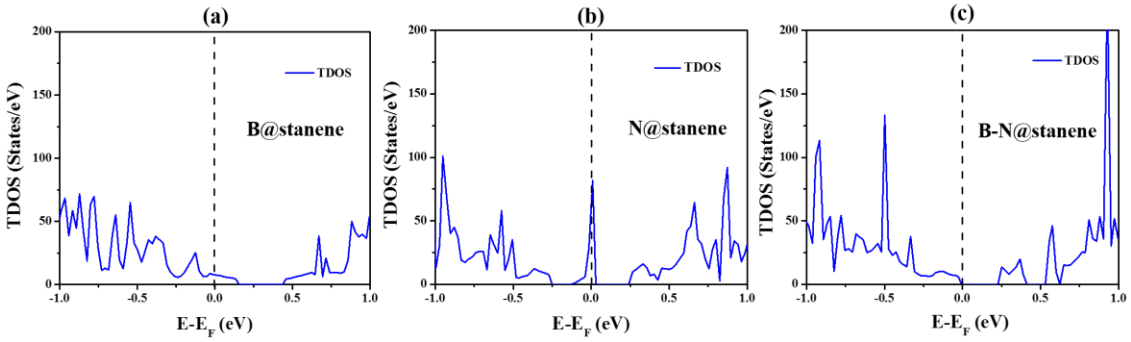


**Figure S3:** TDOS (total density of states) of (a)B@stanene, (b)N@stanene, and (c) 4%B-N@stanene (pattern-a) using HSE06 level of theory. The Fermi level is shifted to zero and indicated by a black dashed line.

**Text S1.** Formation Energy (Ef)/supercell Calculation:

The formation energies ($E_f$) for mono- (B@, and N@) and co-doped B-N@) stanene systems are calculated as follows:

$$E_f = [E_{B/N@stanene} - E_{stanene}] - x[E_{B/N} - E_{Sn}] \quad (1)$$

$$E_f = [E_{B-N@stanene} - E_{stanene}] - x[E_B + E_N] - 2E_{Sn} \quad (2)$$

where, $E_{B/N@stanene}$, $E_{B-N@stanene}$ are the energy of mono doped and co-doped stanene and $E_{stanene}$ is the energy of pure stanene. $E_{B/N}$, $E_{Sn}$ are the chemical potential of dopant (B and N) and Sn atom respectively. $E_B$ and $E_{Sn}$ are calculated from the most stable bulk structure of α-rhombohedral boron and α-Sn, respectively. $E_N$ is calculated from the total energy of $N_2$ molecule.

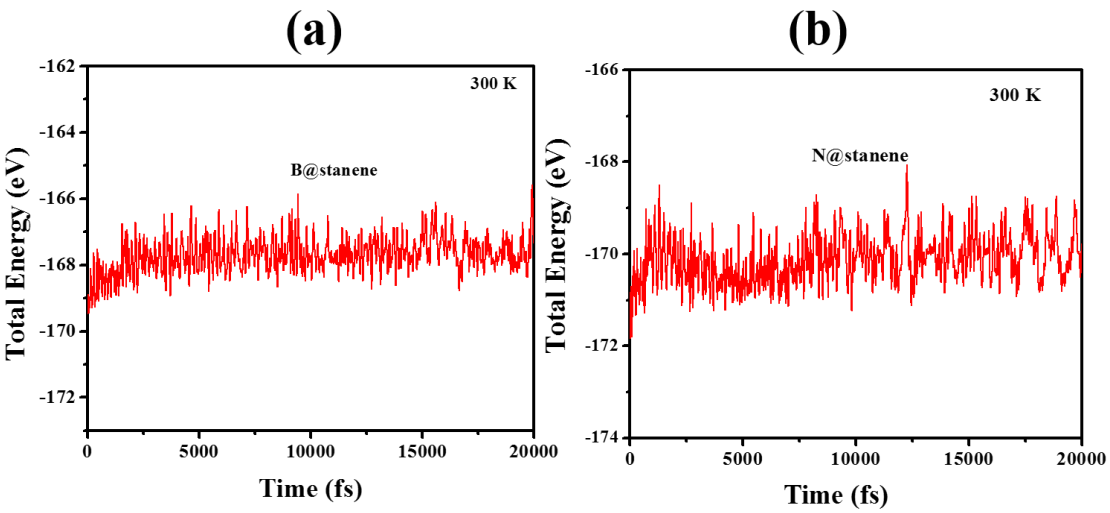


**Figure S4:** Total energy fluctuation during AIMD simulations of (a) B@stanene and (b) N@stanene at 300K temperature.

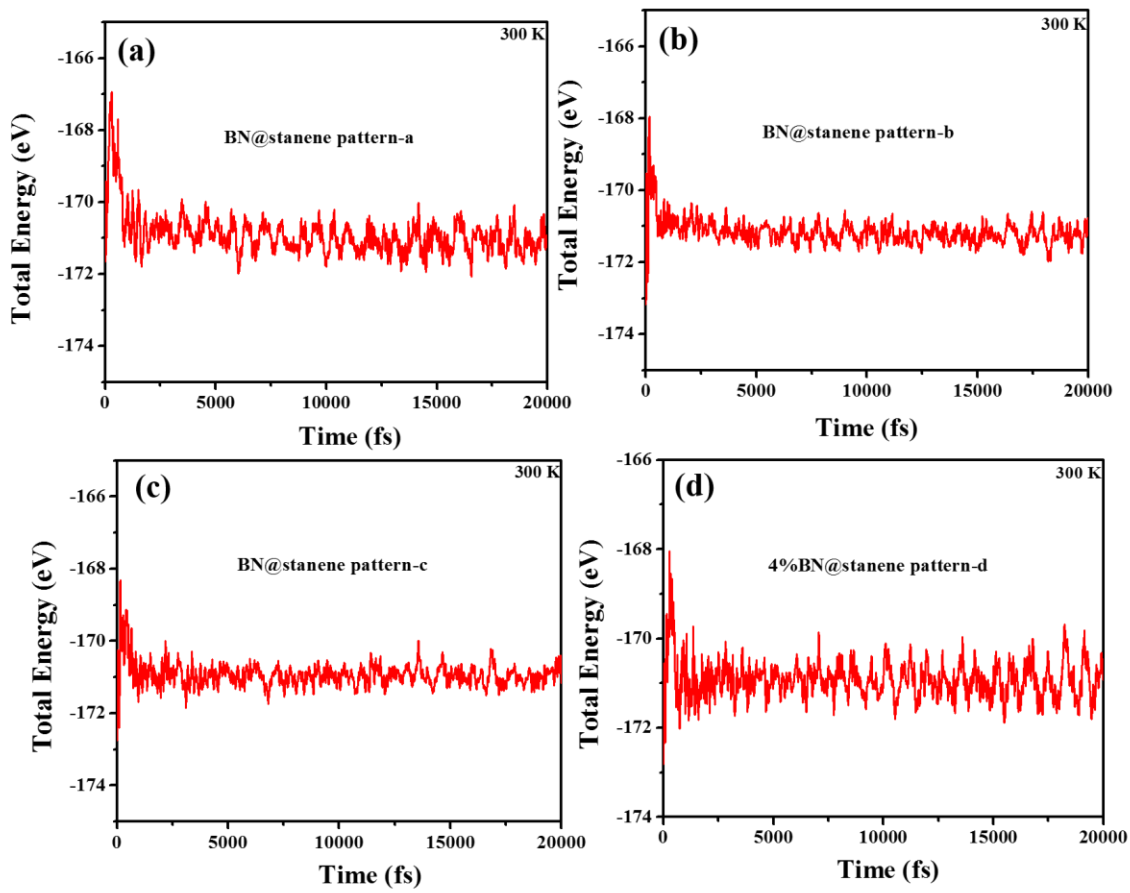


**Figure S5:** Total energy fluctuation during AIMD simulations of different doped system; (a) pattern-a; (b) pattern-b; (c) pattern-c and (d) pattern-d, respectively at 300K temperature.

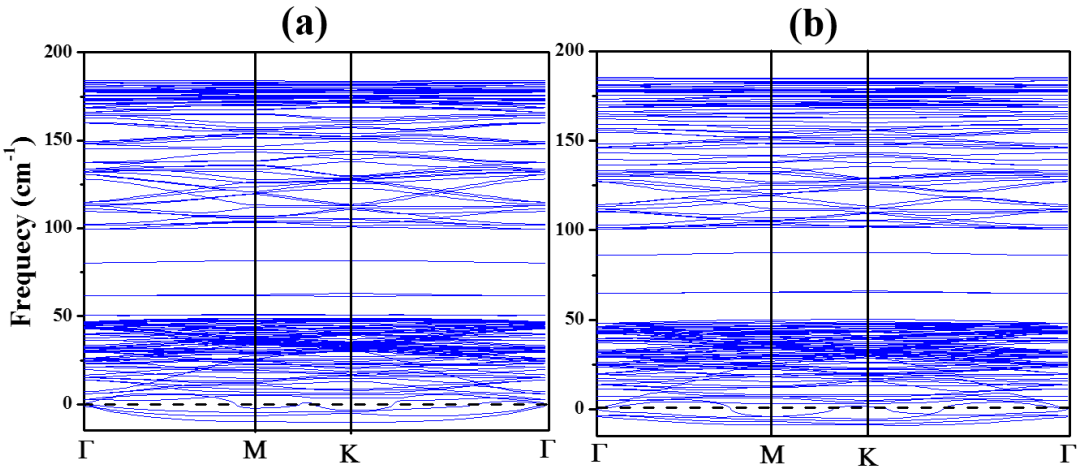


**Figure S6:** Phonon dispersion of 5×5 supercell (50 atoms) of (a) B@, and (b) N@stanene.

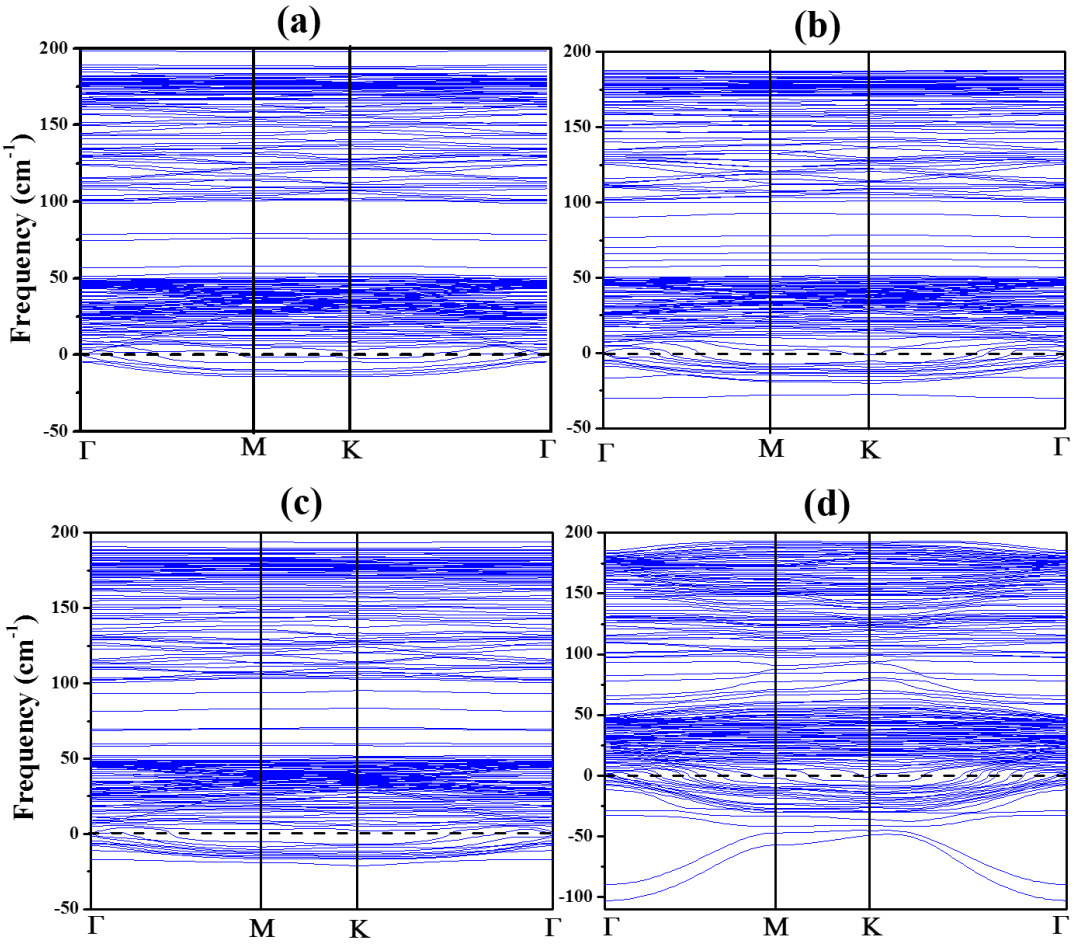


**Figure S7:** Phonon dispersion of 5×5 supercell (50 atoms) of 4%B-N@stanene: (a) pattern-a without any symmetry constraint; (b) pattern-b; (c)pattern-c and (d)pattern-d, respectively.

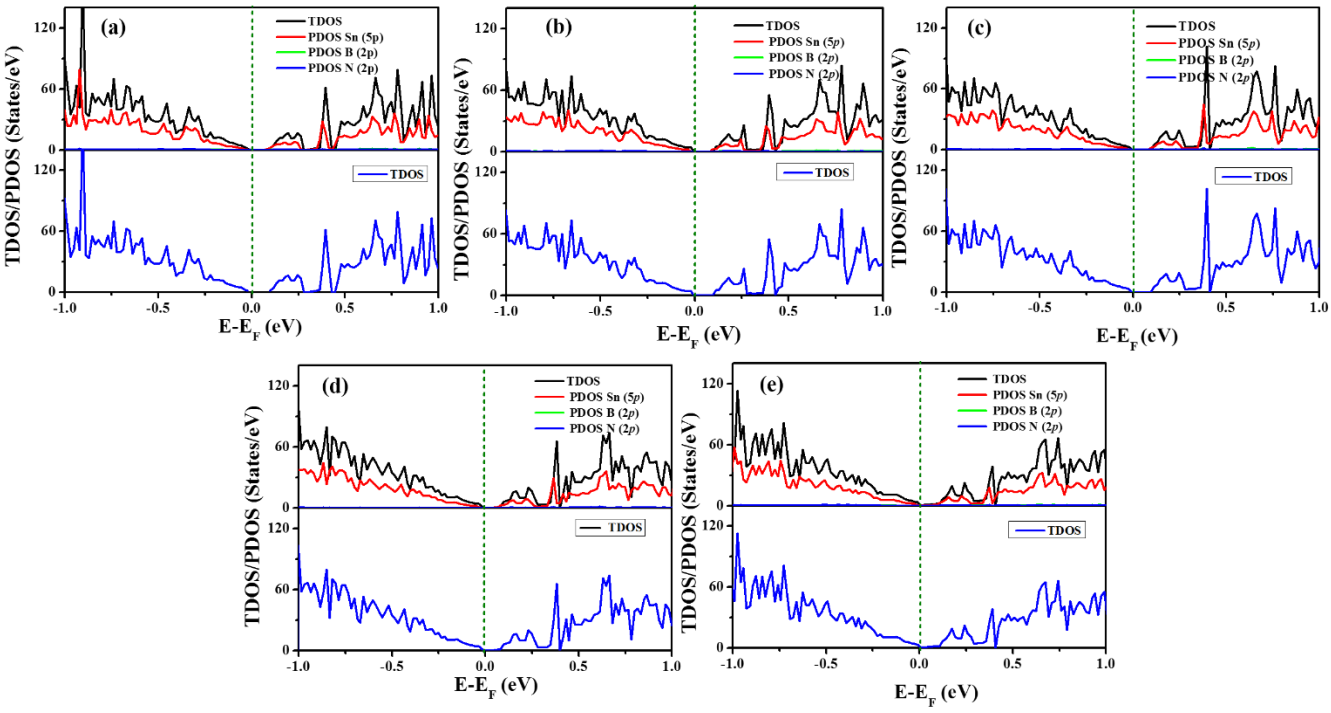


**Figure S8:** TDOS and PDOS of 4%BN@stanene (pattern-a) after different uniaxial tensile strain of 1% to5% represented in figure from (a) to (e). The Fermi level is shifted to zero and indicated by a green dashed line.

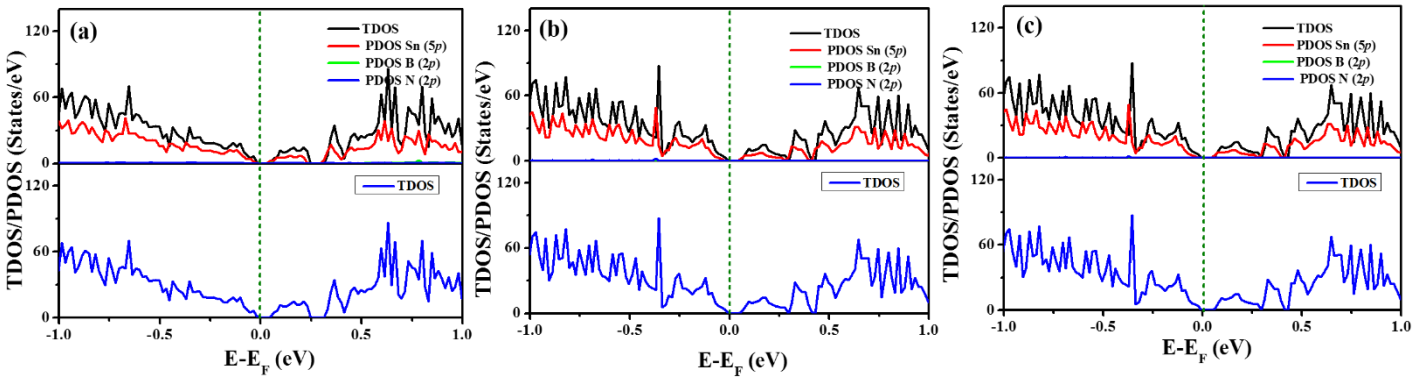


**Figure S9:** TDOS and PDOS of 4%BN@stanene (pattern-a) after different uniaxial compressive strain of 3-5% represented in figure from (a) to (c). Here, the Fermi level is shifted to zero and indicated by a green dashed line.

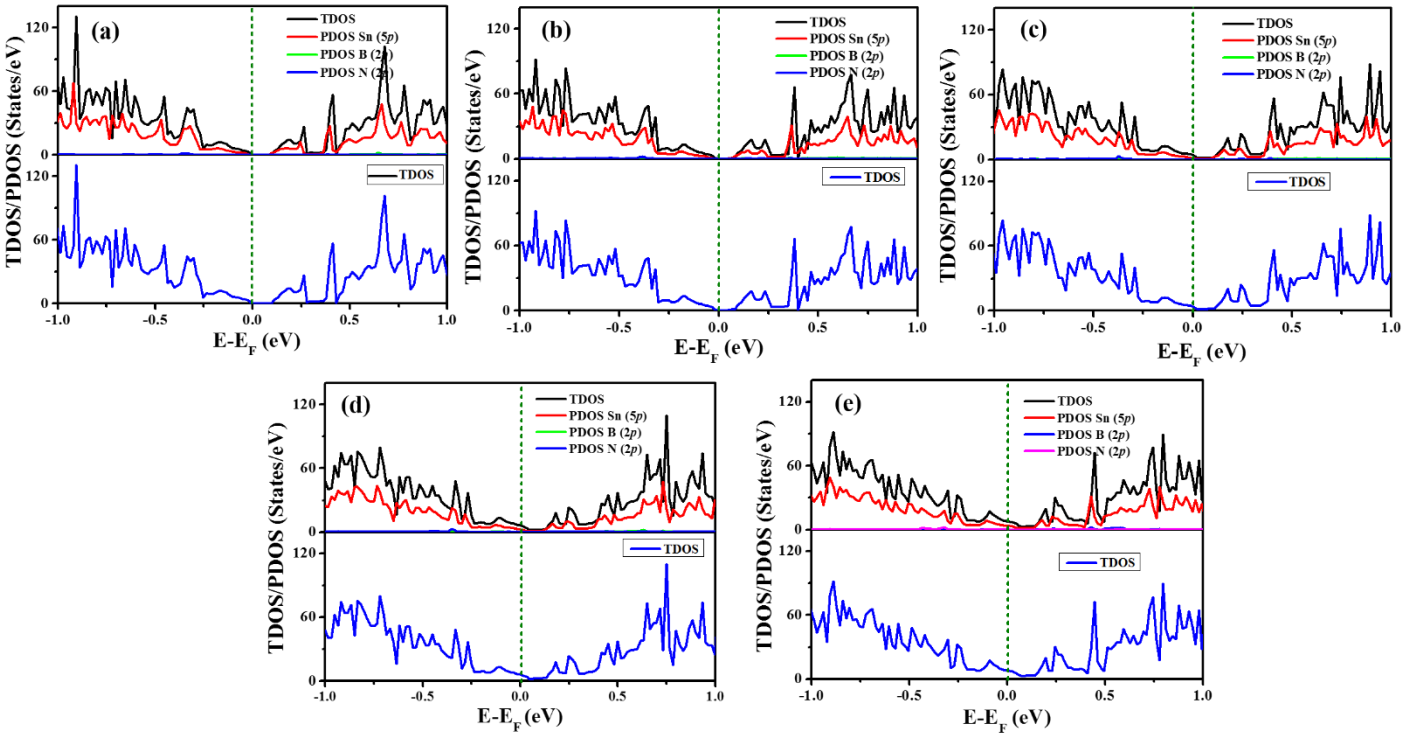


**Figure S10:** TDOS and PDOS of 4%BN@stanene (pattern-a) after different biaxial tensile strain of 1% to5% represented in figure from (a) to (e). Here the Fermi level is shifted to zero and indicated by a green dashed line.

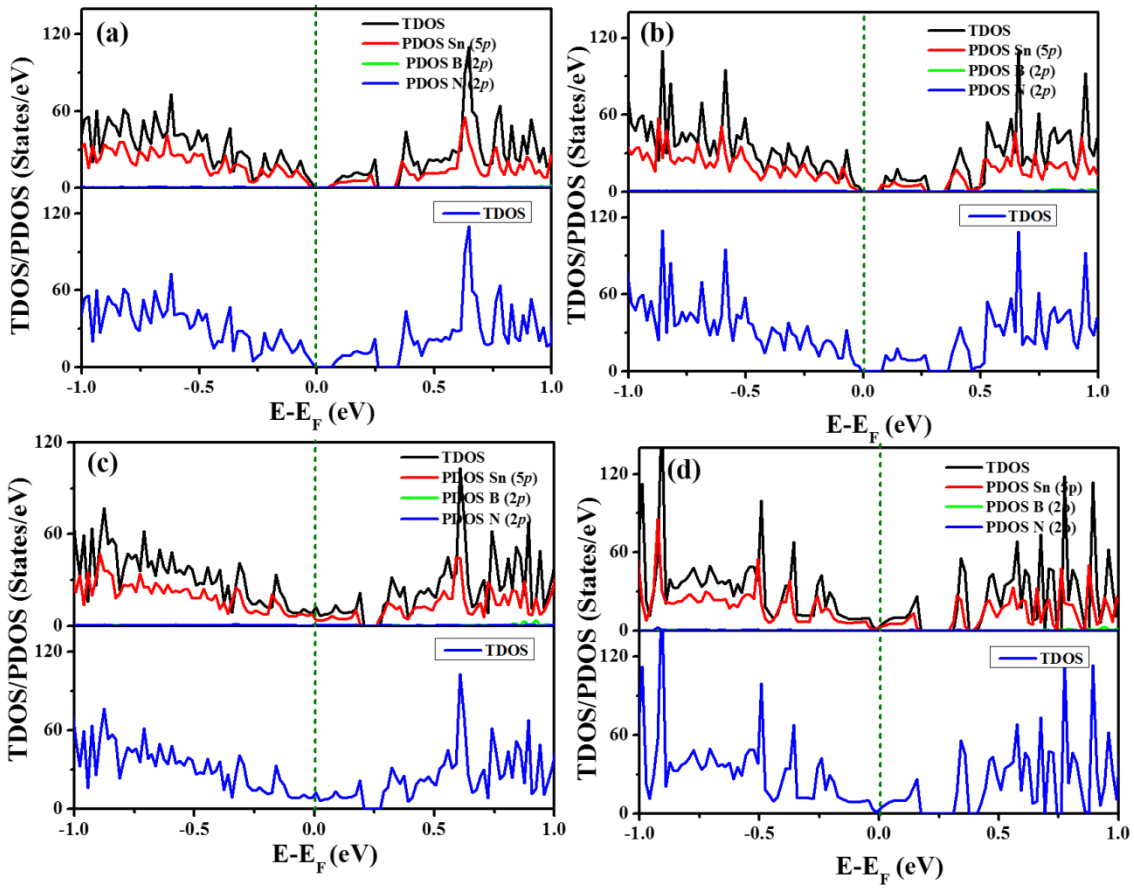


**Figure S11:** TDOS and PDOS of 4%BN@stanene (pattern-a) after different biaxial compressive strain of 2% to5% represented in figure from (a) to (d). Here the Fermi level is shifted to zero and indicated by a green dashed line.

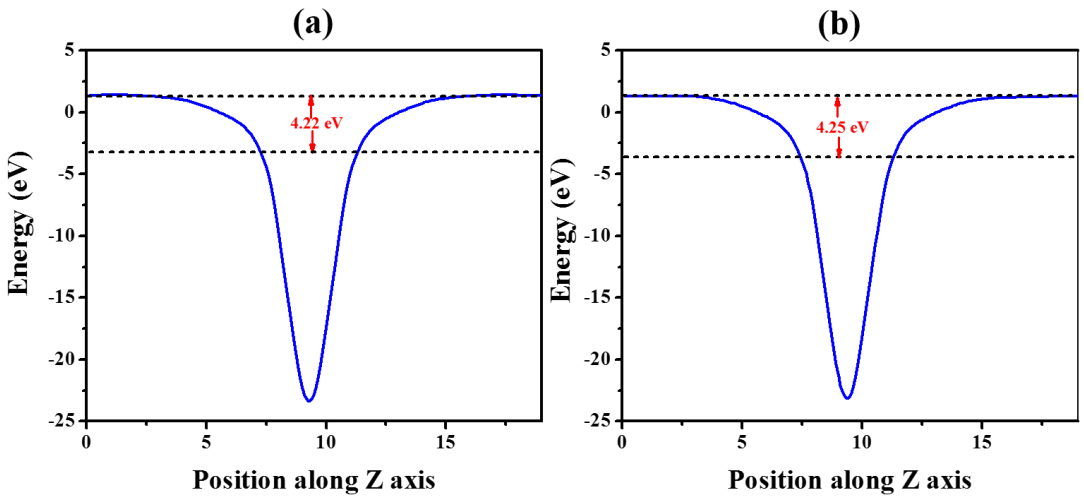


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**Table S1:** Band gap ($E_g$) value with uniaxial and biaxial tensile and compressive strain of 4%BN@stanene (pattern-a) and their bond length after strain [Sn-N bond length given in parenthesis ($d_{Sn-N}$)] and buckling height (h).

| % Strain | $E_g$ (eV) | | $d_{Sn-B}$ ($d_{Sn-N}$) | | h(Å) | |
|---|---|---|---|---|---|---|
| | Uniaxial | Biaxial | Uniaxial | Biaxial | Uniaxial | Biaxial |
| -5 | 0.08 | 0.00 | 2.16 (2.00) | 2.14 (2.00) | 3.33 | 4.83 |
| -4 | 0.08 | 0.00 | 2.16 (2.00) | 2.16 (2.01) | 2.67 | 1.68 |
| -3 | 0.06 | 0.10 | 2.17 (2.01) | 2.16 (2.00) | 1.34 | 4.32 |
| -2 | 0.13 | 0.08 | 2.17 (2.00) | 2.17 (2.01) | 1.13 | 1.57 |
| -1 | 0.13 | 0.13 | 2.18 (2.01) | 2.17 (2.00) | 1.16 | 1.58 |
| 0 | 0.08 | 0.08 | 2.18 (2.01) | 2.18 (2.01) | 1.09 | 1.09 |
| 1 | 0.10 | 0.12 | 2.18 (2.01) | 2.19 (2.01) | 1.08 | 1.14 |
| 2 | 0.12 | 0.05 | 2.19 (2.01) | 2.20 (2.01) | 1.14 | 1.10 |
| 3 | 0.12 | 0.00 | 2.19 (2.01) | 2.21 (2.01) | 1.12 | 1.07 |
| 4 | 0.05 | 0.00 | 2.20 (2.01) | 2.22 (2.01) | 1.14 | 1.02 |
| 5 | 0.00 | 0.00 | 2.20 (2.01) | 2.22 (2.00) | 1.12 | 0.98 |