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

Electronic Supplementary Information (ESI)

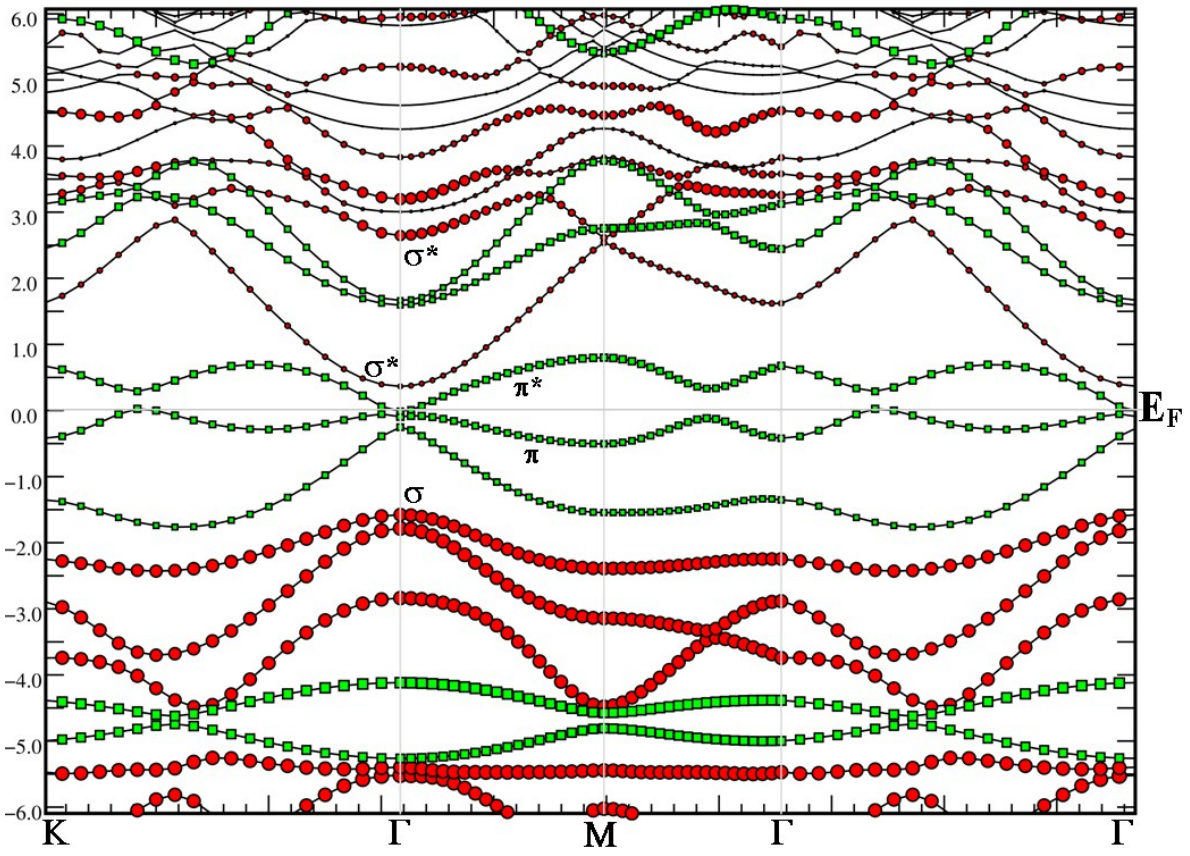

Figure S1. The orbital contributions of atoms in electronic band structure of planar Si_2BN. The (s, p_x, p_y) orbitals combine to form the in-plane σ (bonding nature in valence band) and $\sigma*$ (anti-bonding in conduction band) and it's shows red circle. The p_z orbitals shows green square creates the delocalized π (bonding) and $\pi*$ (anti-bonding) orbitals.

Table S1: The optimised bond lengths (Å) and angles (º) between atoms in Si_2BN monolayer system with applying external electric field at 5 V/nm and 10 V/nm.

Properties/Sr. No.	Pure Si_2BN	5 V/nm	10 V/nm
Bond lengths (Å)	B-N=1.465 Si-N=1.756 Si-B=1.953 Si-Si=2.244	B-N=1.461 Si-N=1.752 Si-B=1.953 Si-Si=2.256	B-N=1.439 Si-N=1.743 Si-B=1.968 Si-Si=2.267
Angles (°)	Si-B-Si=112.82 B-Si-N=118.41 Si-N-Si=123.99 Si-Si-B=123.59 B-N-Si=118 Si-Si-N=118 N-B-Si=123.59	Si-B-Si=112.99 B-Si-N=118.64 Si-N-Si=124.29 Si-Si-B=123.51 B-N-Si=117.85 Si-Si-N=117.85 N-B-Si=123.51	Si-B-Si=112.28 B-Si-N=118.40 Si-N-Si=124.53 Si-Si-B=123.86 B-N-Si=117.74 Si-Si-N=117.74 N-B-Si=123.86

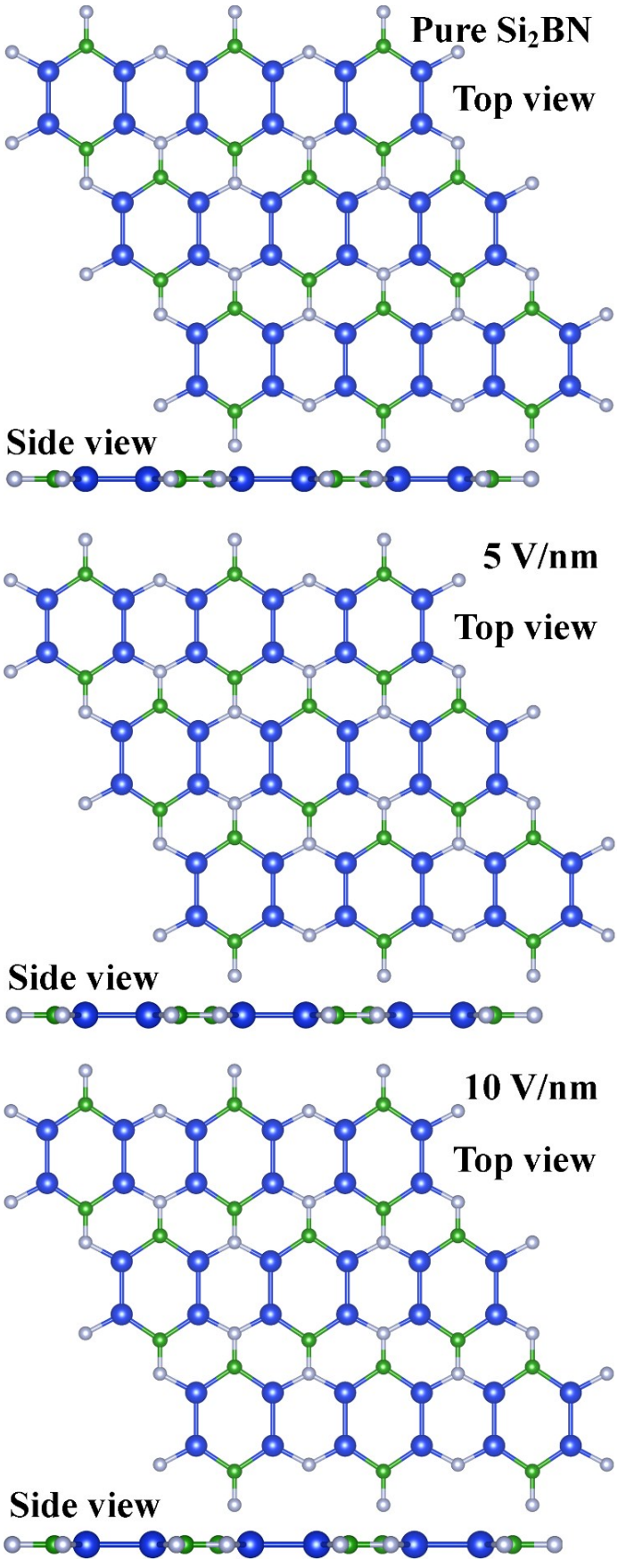

Figure S2: The optimised structures of Si_2BN monolayer with applying external electric field at 5 V/nm and 10 V/nm.