SUPPLEMENTARY INFORMATION

Electrically Tunable Band Gap in Strained h-BN/Silicene van der Waals Heterostructures

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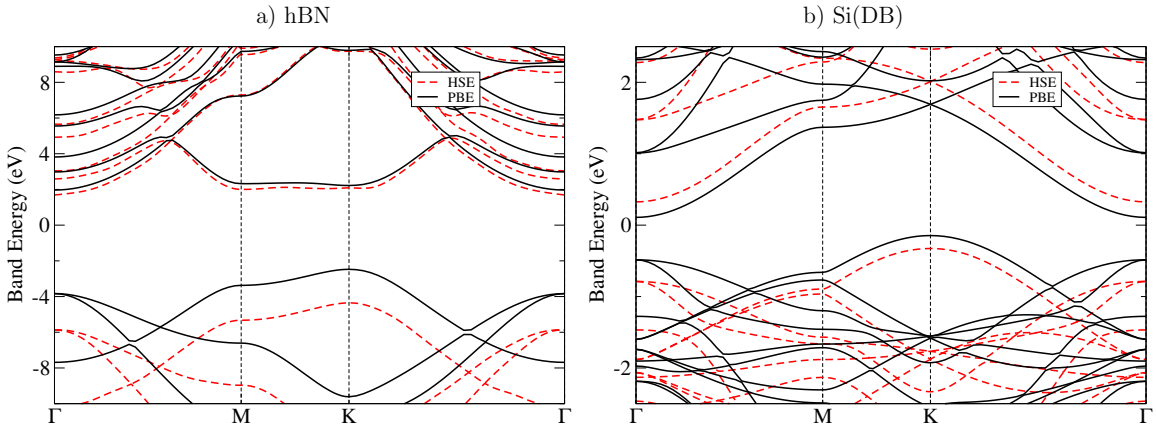

Figure S1: Electronic band strucutres for (a) hBN and (b) Si(DB) using PBE (black lines) and HSE06 (red dashed lines) exchange-correlation functionals.

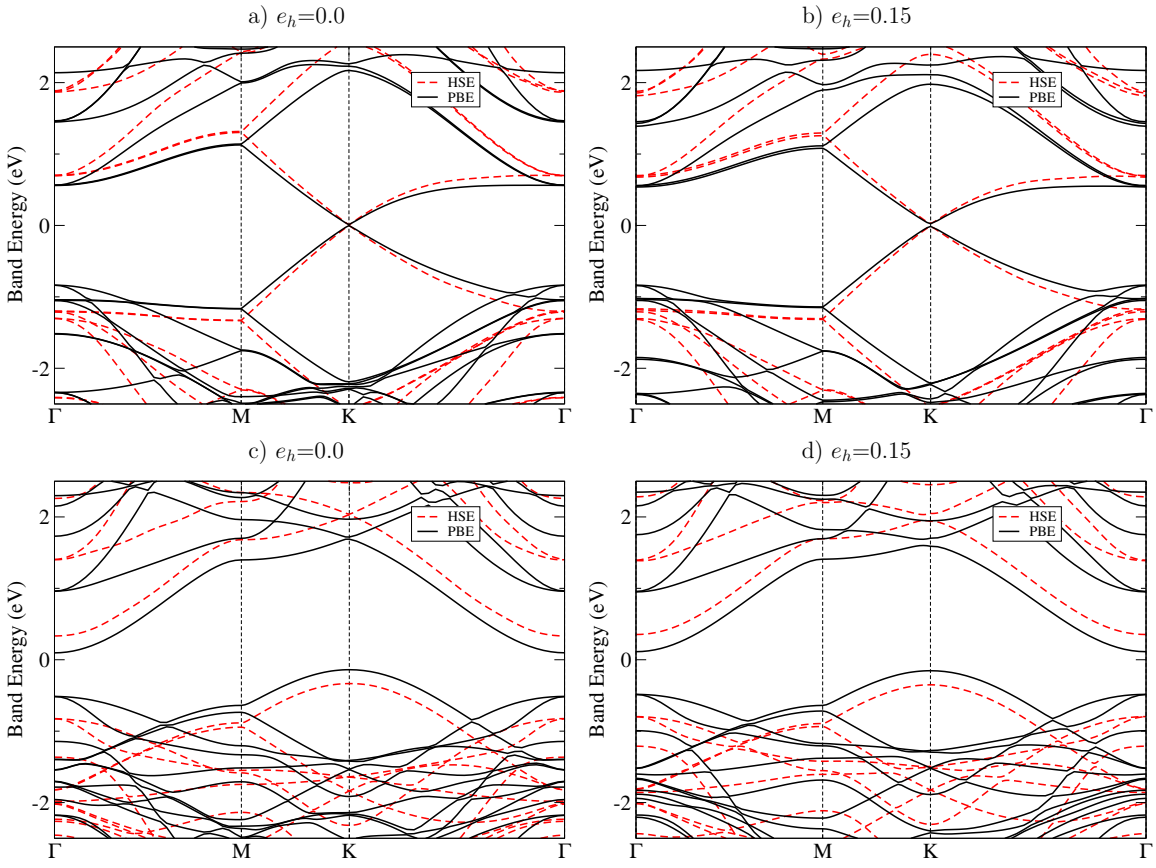

Figure S2: Electronic band structures for h-BN/Si(LB) (top panels) and h-BN/Si(DB) (bottom panels) at equilibrium position (figures (a) and (c), respectively) and under vertical strain figures (b) and (d), respectively. Black lines and red dashed lines are PBE and HSE06 exchange-correlation functionals.

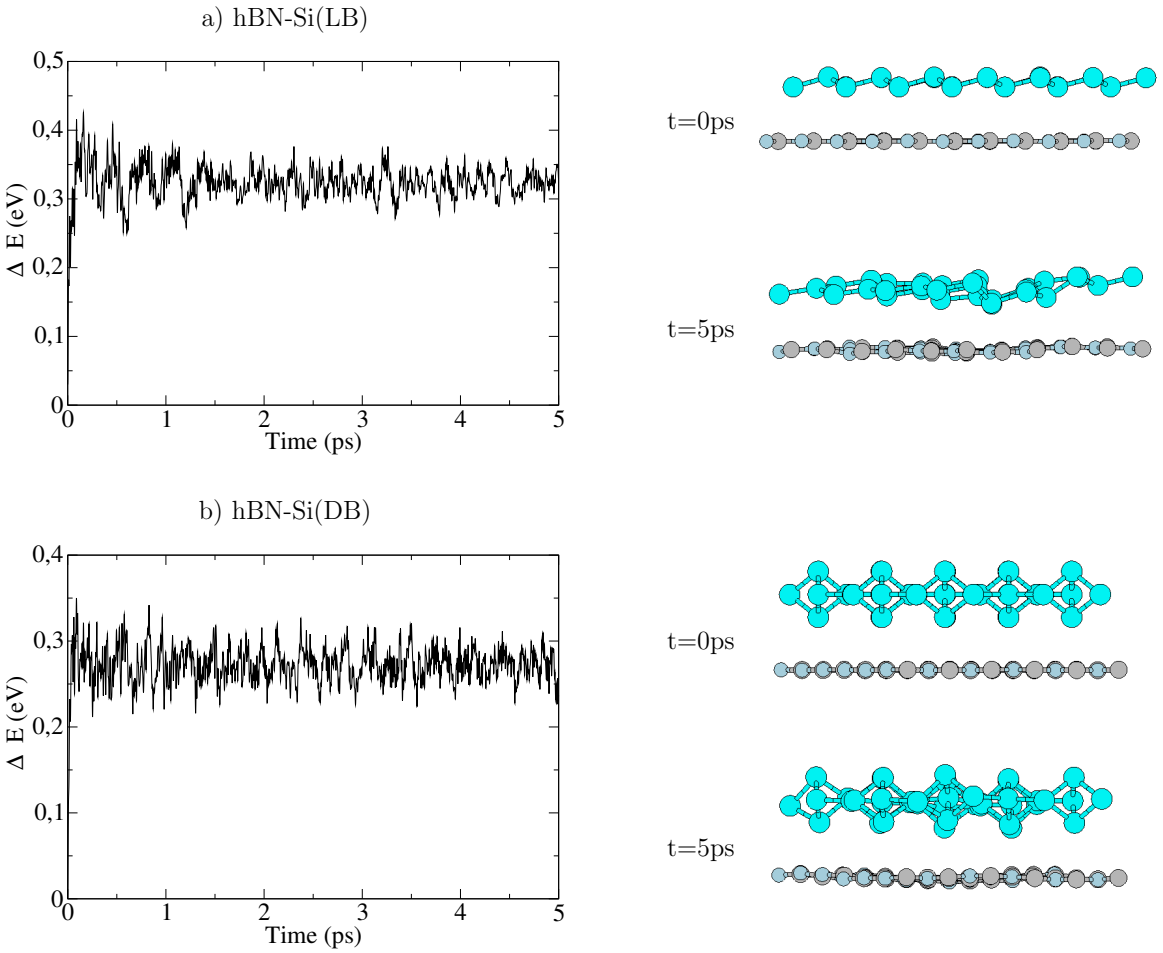

Figure S3: Variation of the total energy vs. time and the initial and final snapshots of AIMD simulations of (a) h-BN/Si(LB) and (b) h-BN/Si(DB). 5 ps simulations were conducted in the NVT ensemble at T = 300 K and a timestep of 1 fs.

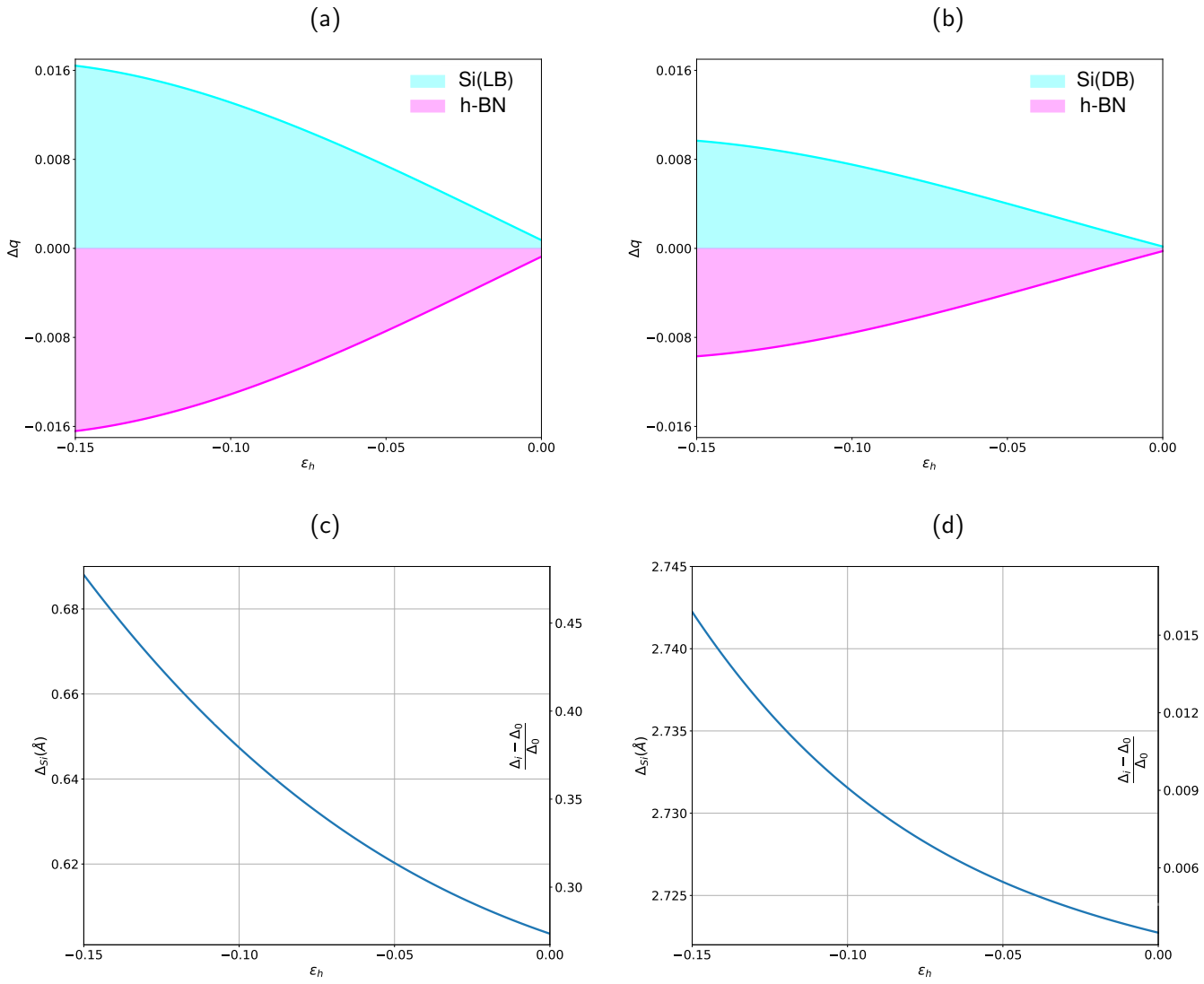

Figure S4: The charge transfer from h-BN to (a) Si(LB) and (b) Si (DB) and the buckling height's evolution (Δ_{Si-Si}) as a function of the vertical strain (ε_h) for (c) Si(LB) and (d) Si (DB).

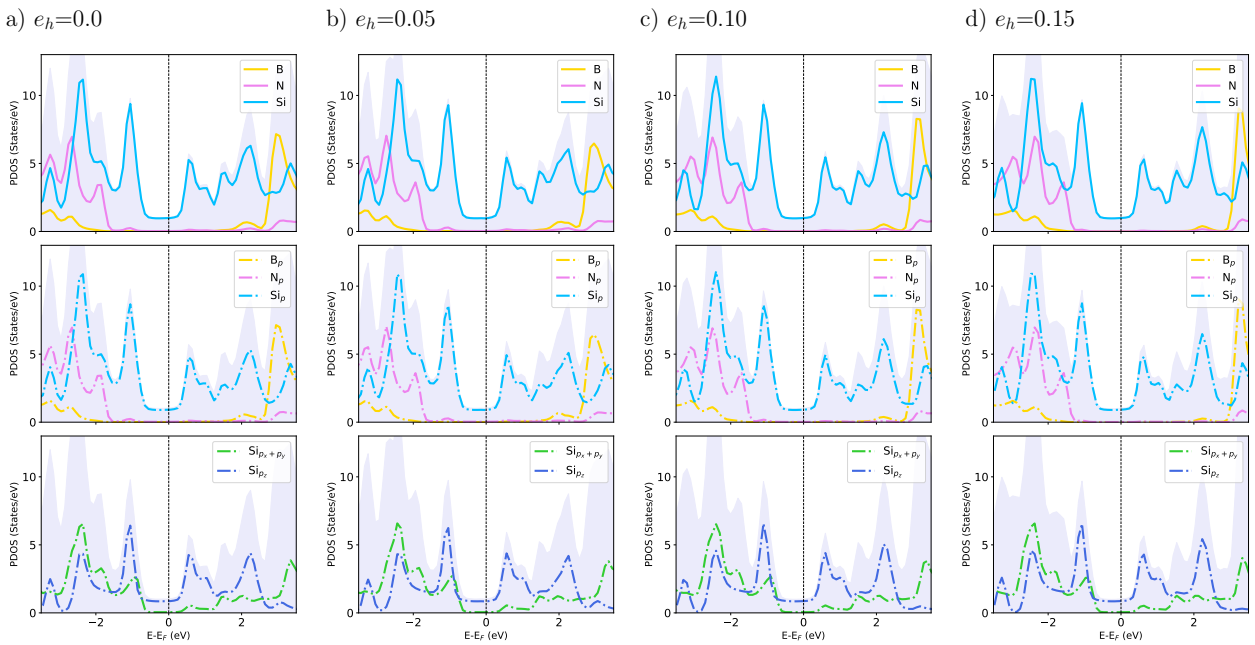

Figure S5: Projected density of states of h-BN/Si(LB) under vertical compression (ε_h) over atom (top panel), over p-orbital (middle painel), and over planar ($p_x + p_y$) and perpendicular (p_z) $p-$orbitals of Si (bottom painel).

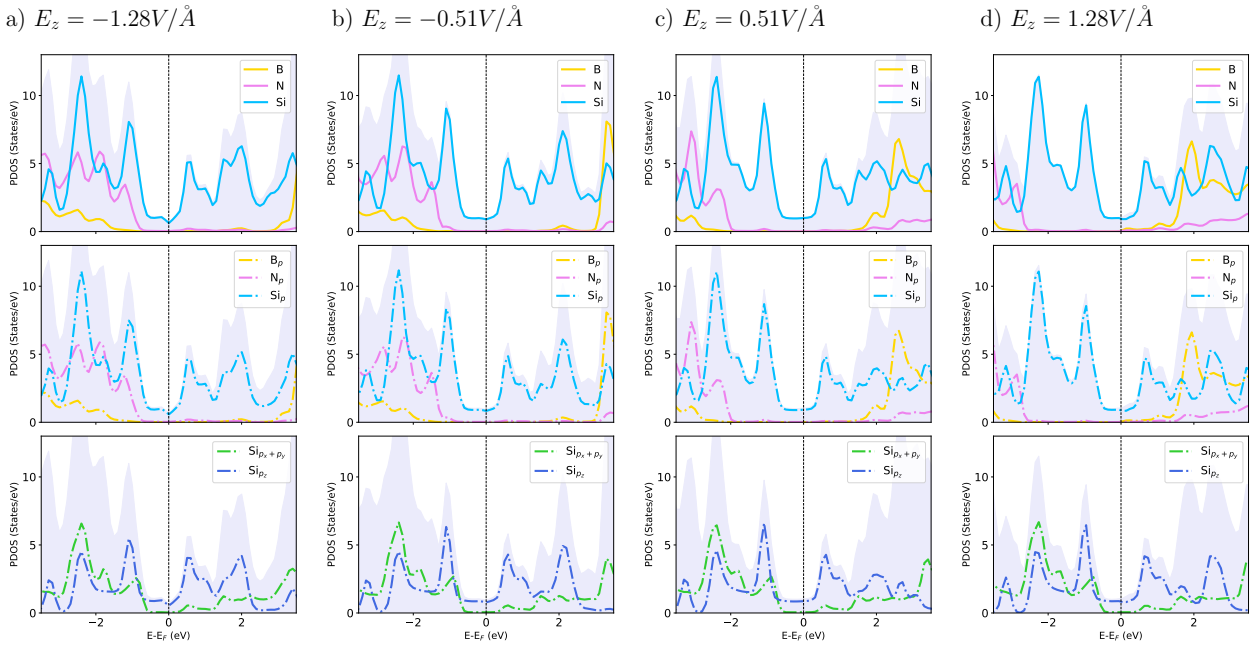

Figure S6: Projected density of states of h-BN/Si(LB) under external electric field (E_z) over atom (top panel), over p-orbital (middle painel), and over planar ($p_x + p_y$) and perpendicular (p_z) $p-$orbitals of Si (bottom painel).

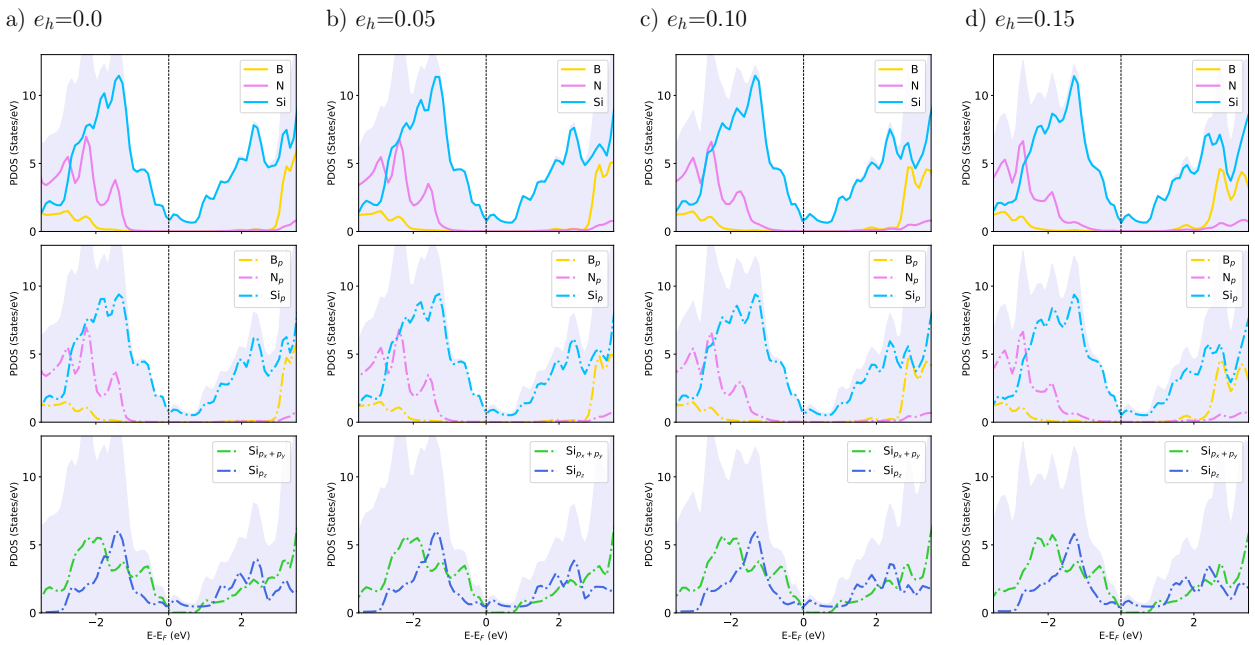

Figure S7: Pojetcted density of states of h-BN/Si(DB) under vertical compression (ε_h) over atom (top panel), over p-orbital (middle painel), and over planar ($p_x + p_y$) and perpendicular (p_z) $p-$orbitals of Si (bottom painel).

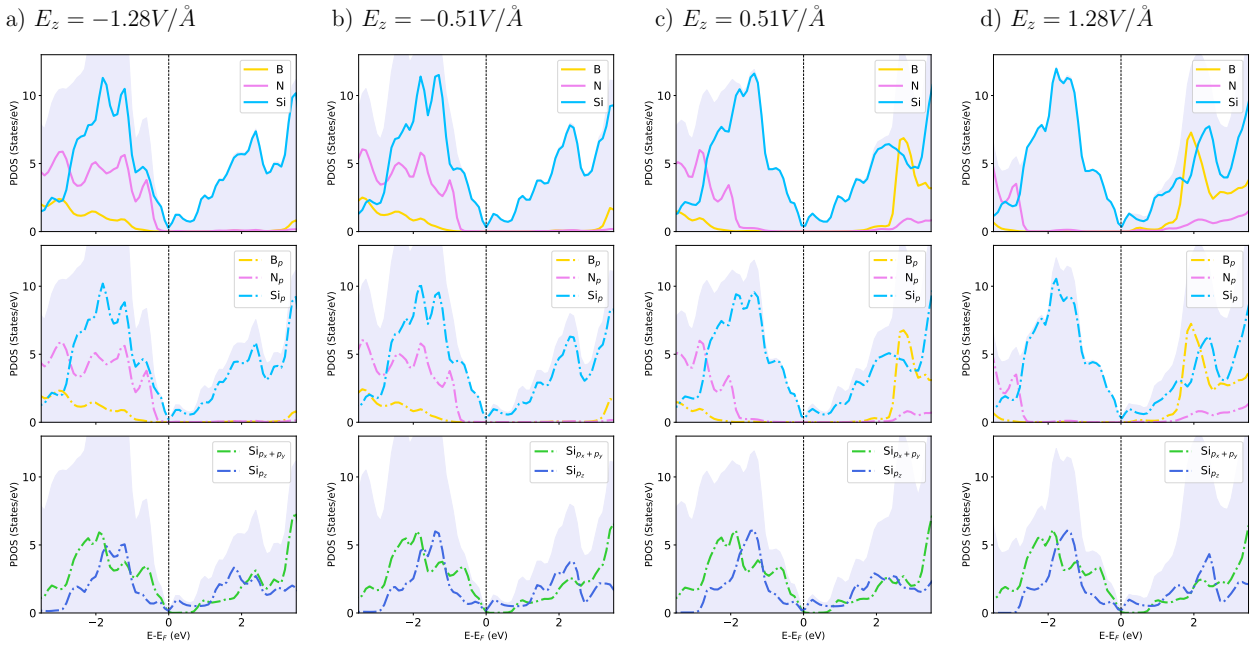

Figure S8: Projected density of states of h-BN/Si(DB) under under external electric field (E_z) over atom (top panel), over p-orbital (middle painel), and over planar ($p_x + p_y$) and perpendicular (p_z) $p-$orbitals of Si (bottom painel).

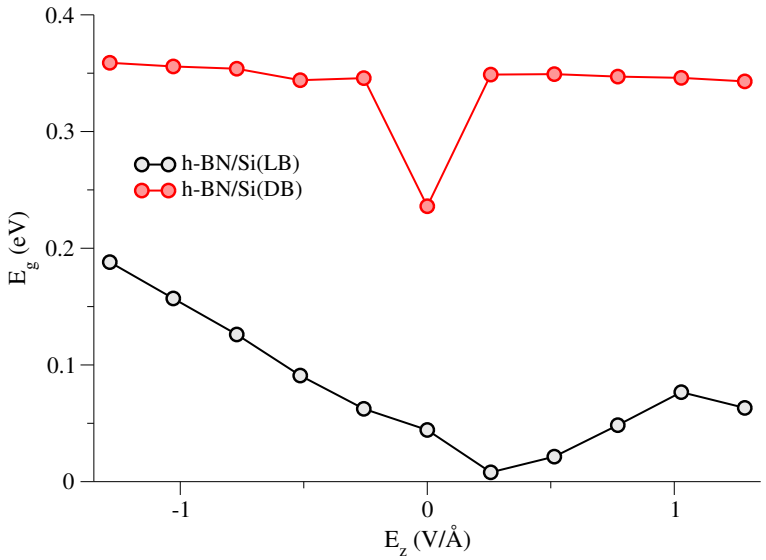

Figure S9: Field dependence of the band gap for h-BN/Si(LB) (black circles) and h-BN/Si(DB) (red circles). Note: there is a transition from direct (K-K) to indirect (K-Gamma) band gap in h-BN/Si(LB) at E_z=1.28eV/$\mathring{A}$.