SUPPLEMENTARY INFORMATION

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

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Figure S1: Electronic band structures 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 ($\Delta_{Si-Si}$) as a function of the vertical strain ($\varepsilon_h$) for (c) Si(LB) and (d) Si (DB).
Figure S5: Projected density of states of h-BN/Si(LB) under vertical compression ($\varepsilon_p$) over atom (top panel), over $p$-orbital (middle panel), and over planar ($p_x + p_y$) and perpendicular ($p_z$) $p$–orbitals of Si (bottom panel).

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

Figure S8: Projected density of states of h-BN/Si(DB) under external electric field ($E_z$) over atom (top panel), over $p$-orbital (middle panel), and over planar ($p_x + p_y$) and perpendicular ($p_z$) $p$-orbitals of Si (bottom panel).
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 $E_z = 1.28$ eV/Å.