Modulation of band gap by applied electric field in Silicene-based hetero bilayers

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Supporting Information

Table-S1: Comparison of present theoretical method with previous work

system	Source	Lattice constant (method)	Band gap	Buckling
graphene	Present work	2.47 Å	~0 eV	0
	S. Tang, J. Yu and L. Liu *Phys. Chem. Chem. Phys.*, **2013** 15, 5067	2.46 Å (PBE+vdw; CASTEP)	~0 eV	0
	Shaoqing Wang *Phys. Chem. Chem. Phys*., **2011**, 13, 11929–11938	2.44 Å (LDA; ABINIT)	~0 eV	0
	H. Sahin, S. Cahangirov, M. Topsakal, E. Bekaroglu, E. Akyurk, R. T. Senger and S. Ciraci, *Phys. Rev. B*:, 2009, 80, 155453	2.46 Å (LDA; VASP)	~0 eV	0
BN monolayer	Present work	2.51 Å	4.45 eV	0
	L. Li, X. Wang, X. Zhao, and M. Zhao, *Phys. Lett A* 2013 377 2628.	2.51 Å (PBE+vdW ; VASP)	-	0
	M. Topsakal, E. Aktürk, and S. Ciraci *Phys. Rev. B* 2009 79 115442.	2.51 Å (PW91-VASP)	4.47 eV	0
	H. Sahin, S. Cahangirov, M. Topsakal, E. Bekaroglu, E. Akyurk, R. T. Senger and S. Ciraci, *Phys. Rev. B*:, 2009, 80, 155453	2.46 Å (LDA; VASP)	4.61eV	0
Silicene	Present work	3.85 Å	~0 eV	0.47 Å
	Shaoqing Wang *Phys. Chem. Chem. Phys*., **2011**, 13, 11929–11938	3.82 Å (LDA; ABINIT)	~0 eV	0.43 Å
	H. Sahin, S. Cahangirov, M. Topsakal, E. Bekaroglu, E. Akyurk, R. T. Senger and S. Ciraci, *Phys. Rev. B*:, 2009, 80, 155453	3.83 Å (LDA; VASP)	~0 eV	0.44 Å
	N. D. Drummond, V. Z´olyomi, and V. I. Fal'ko *Phys. Rev. B* 2012 85, 075423	3.86 Å (PBE; CASTEP)	~0 eV	0.45 Å

Table-S2: Interaction, strain and binding energies of the bilayer systems
(All energies are in unit of **meV/atom**)

	Interaction energy[1]	Strain energy[2]	Binding energy[3#]
Silicene/graphene	-24.6	13.3	-12.7
Silicene/BN	-27.06	4.1	-24.4
Graphene/BN (AB-stacked)	-30.16	5.4	-25.8
Graphene/graphene (AB-stacked)	-24.2	≈0.0	-24.9

1. Interaction energy = $E_{AB}(R=_{optimized})$ - $E_{AB}(R_{interlayer=}\ 8\ Å)$
2. Strain energy = $(E_A + E_B)$ obtained at the bilayer equilibrium configuration
$-(E_A + E_B)$ obtained at the monolayer equilibrium configuration
3. Binding energy (binding energy with respect to the constituent monolayers) $E_{binding} = E_{AB} - E_A - E_B$.

#Theoretical binding energy (Interaction energy + Strain energy) has approximately 6.5% difference with the calculated binding energy. This is due to the long range interaction assessed by vdW correction term (D2) within PBE functional, during estimation of interaction energy, in particular $E_{AB}(R_{interlayer=}\ 8\ Å)$ term. While calculating the binding energy, the two layers have been assumed to be infinitely separated having no interaction at all.

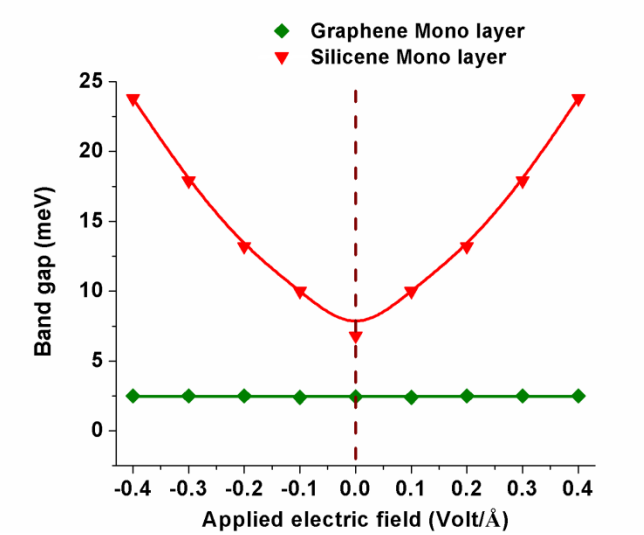

Figure S1: The variation of the band gap with the external perpendicular electric field.

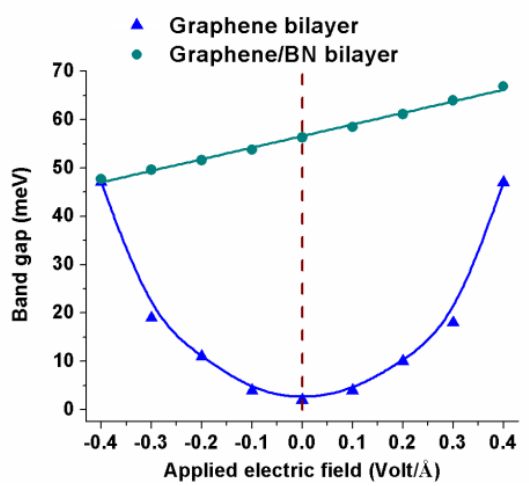

Figure S2: The variation of the band gap with the external perpendicular electric field.

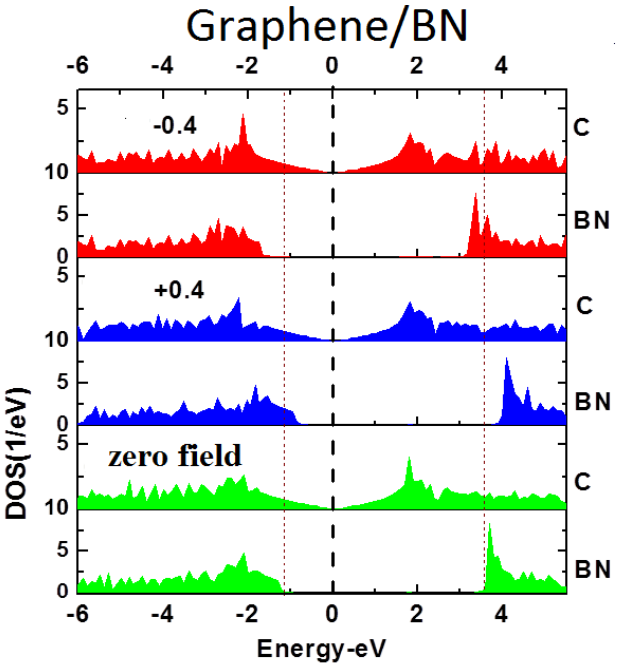

Figure S3: The p_z orbital projected density of states for graphene/BN for E_{Field} = 0, +0.4 V/Å, and -0.4 V/Å, Zero of the energy is aligned to the Fermi level., The dotted line corresponds to the top of the valance and bottom of the conduction band of the BN monolayer layer at E_{Field} = 0.

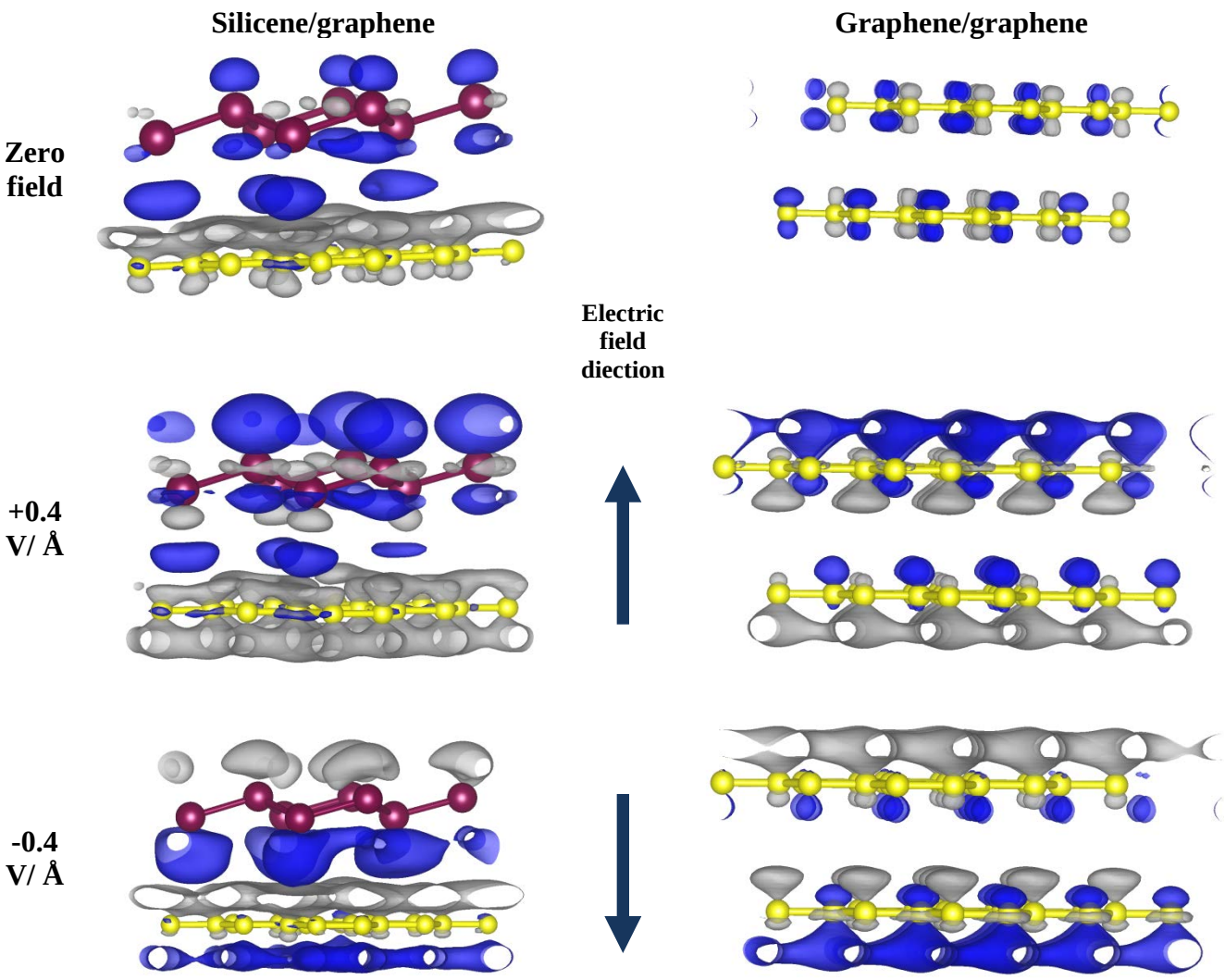

Figure S4: Charge density difference ($\Delta\rho$) for silicene/graphene and graphene/graphene bilayer system in zero applied field and +0.4 V/ Å and -0.4 V/ Å external applied field. The blue lobe indicates increase of charge and gray lobes represented reduction of charge from those sites. Positive value of electric field defines the field from bottom to top. The charge contour value is $6e^{-3}$ electron/bohr^3.

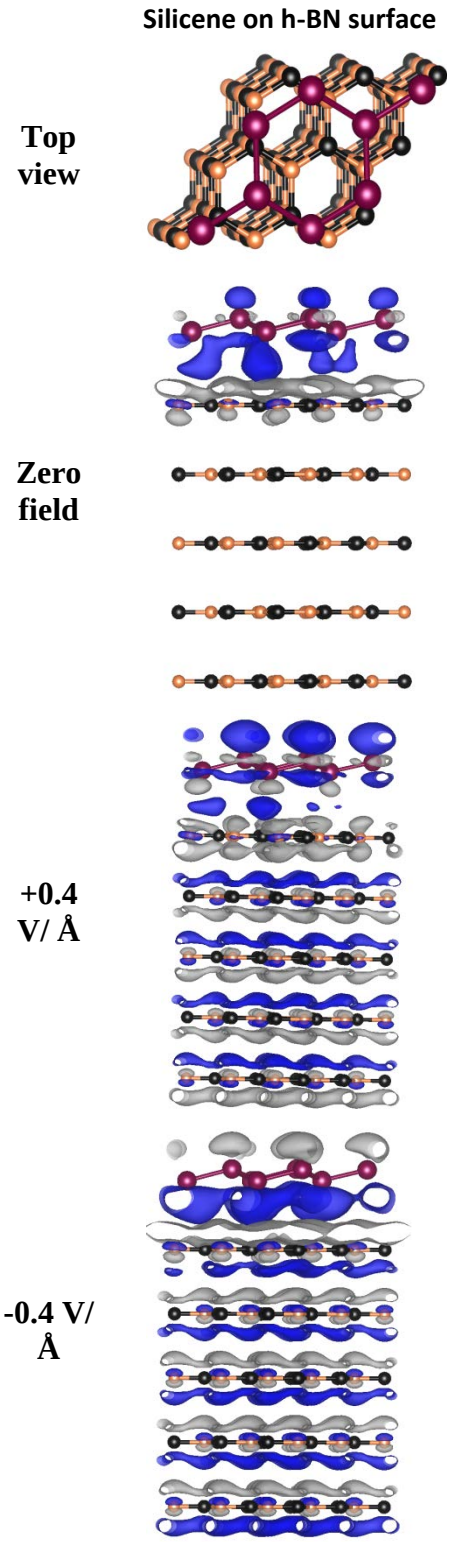

Figure S5: Structure and charge density difference ($\Delta\rho$) for silicene/BN (*Si: purple, B: black , N: Orange*)