Supplementary Information

Title: Bond states, moiré pattern and bandgap modulation of two-dimensional BN/SiC van der Waals heterostructures

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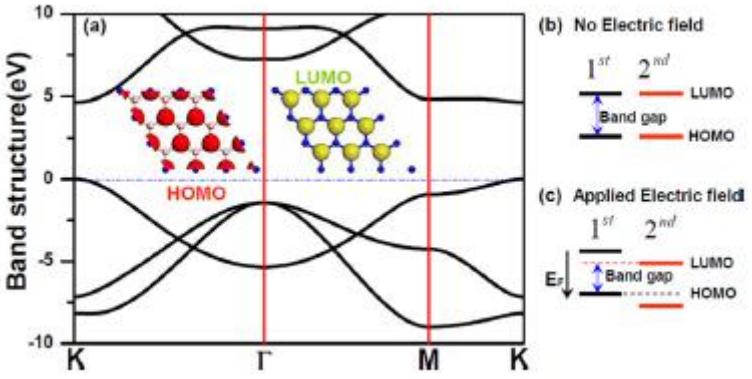
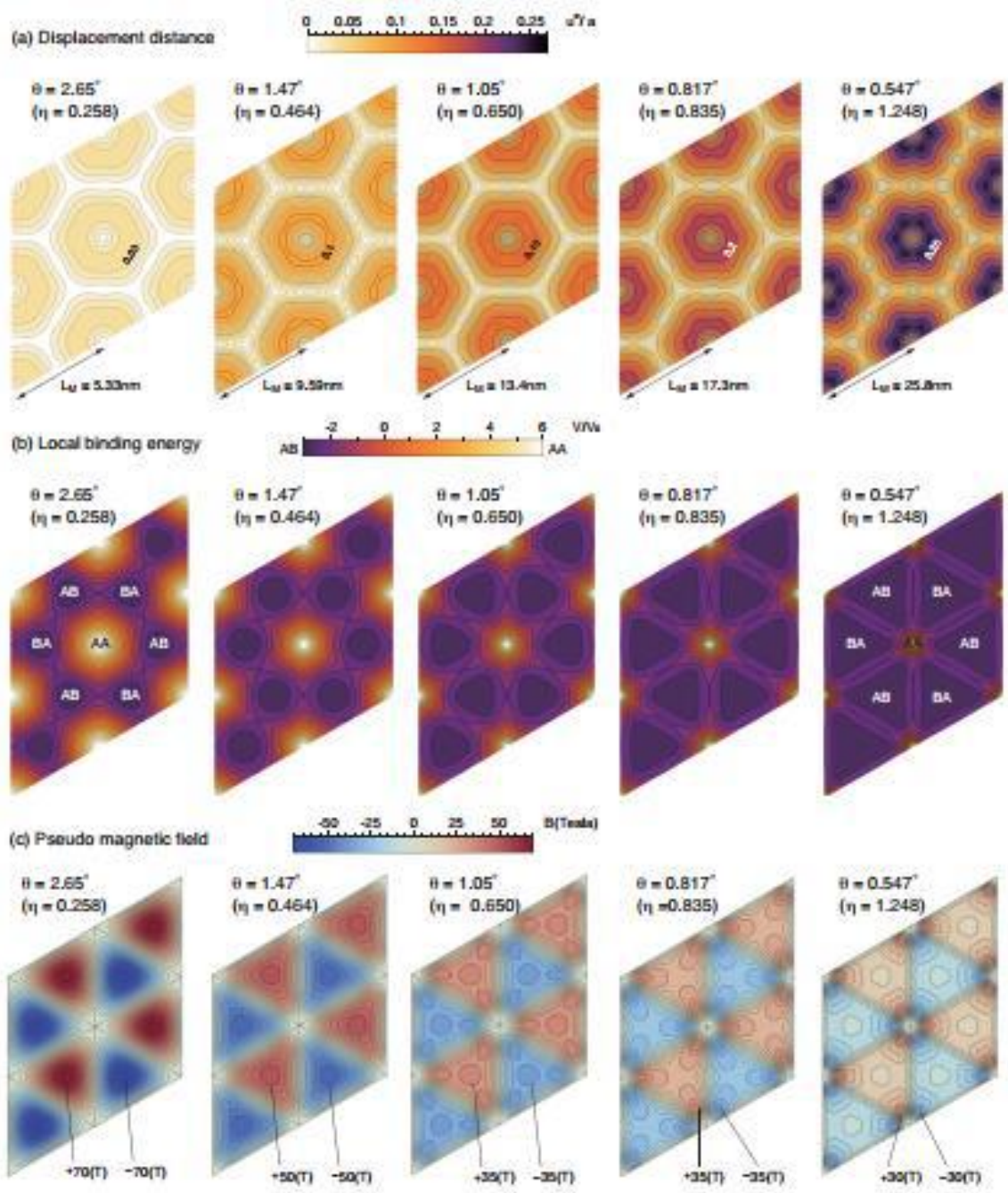


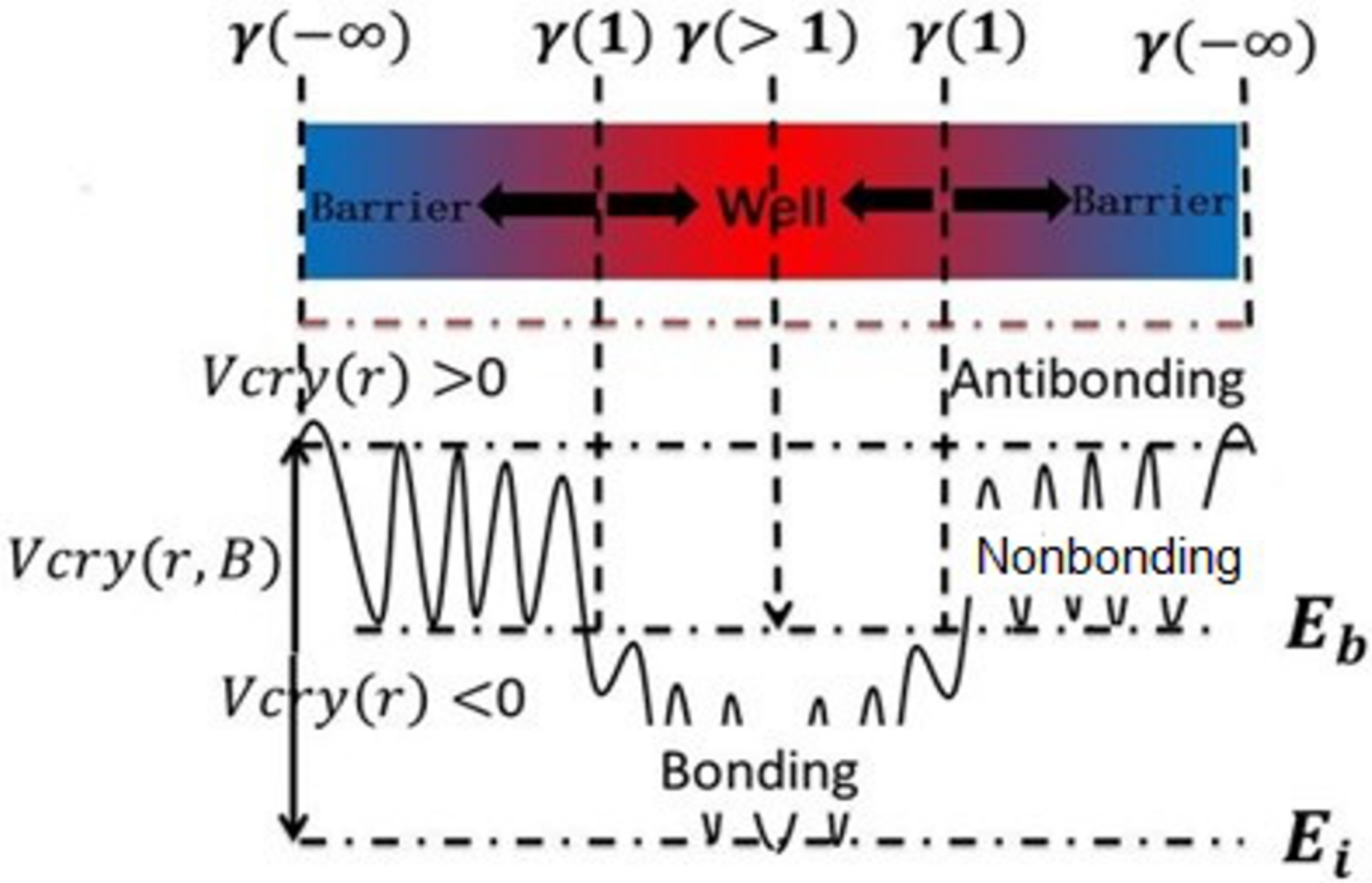
TABLE I. The binding energy E_b, energy difference E_{diff}, BN spacing d, and band gap of different stacking BN bilayers.

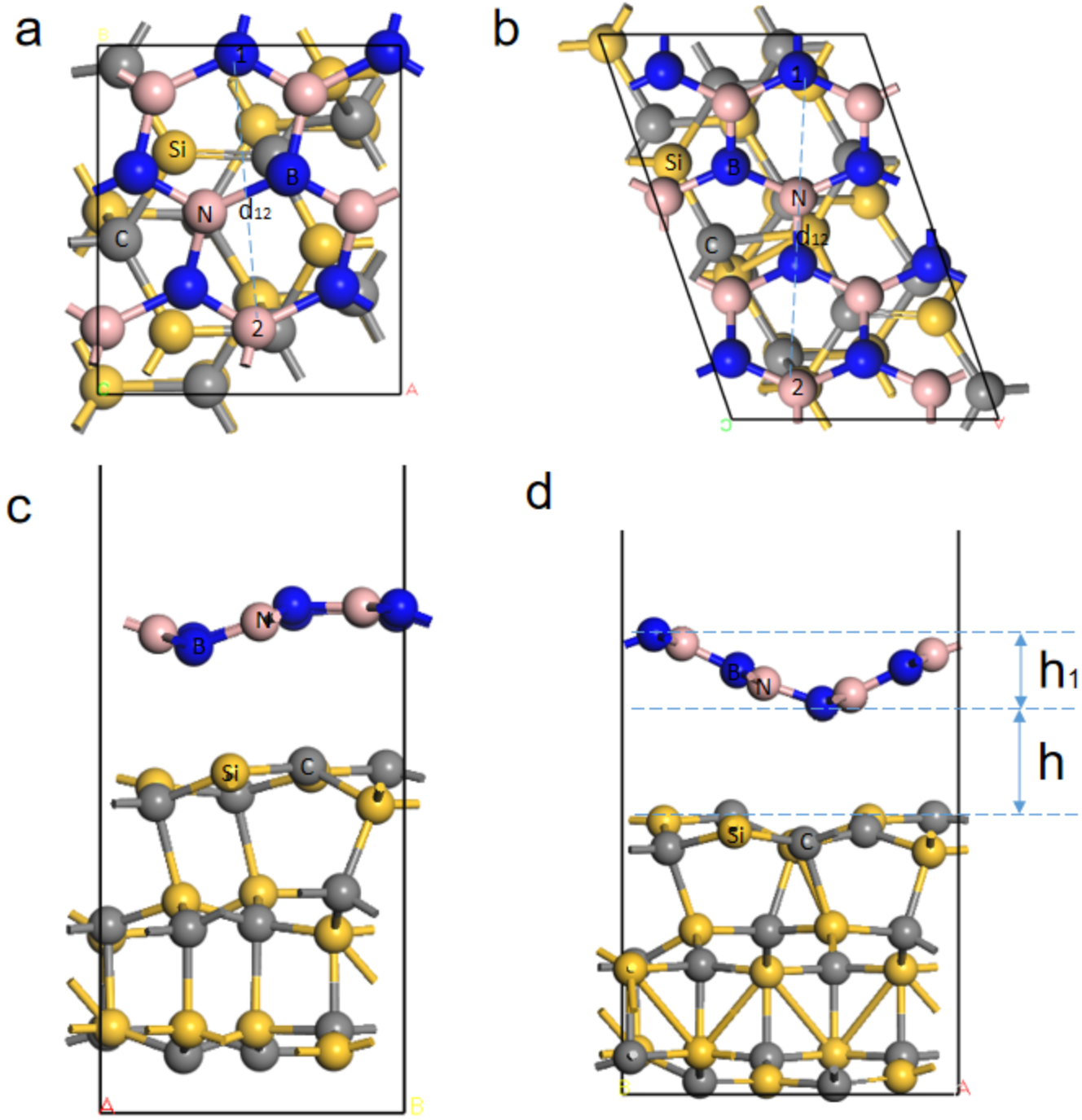
Stacking	E_b (meV)	E_{diff} (meV)	d (Å)	Band gap (eV)
AB	−84	0	3.203	4.44
AA′	−82	2	3.253	4.41
AB′	−73	11	3.206	3.97
AB″	−52	32	3.434	4.03
AA	−45	39	3.497	3.97

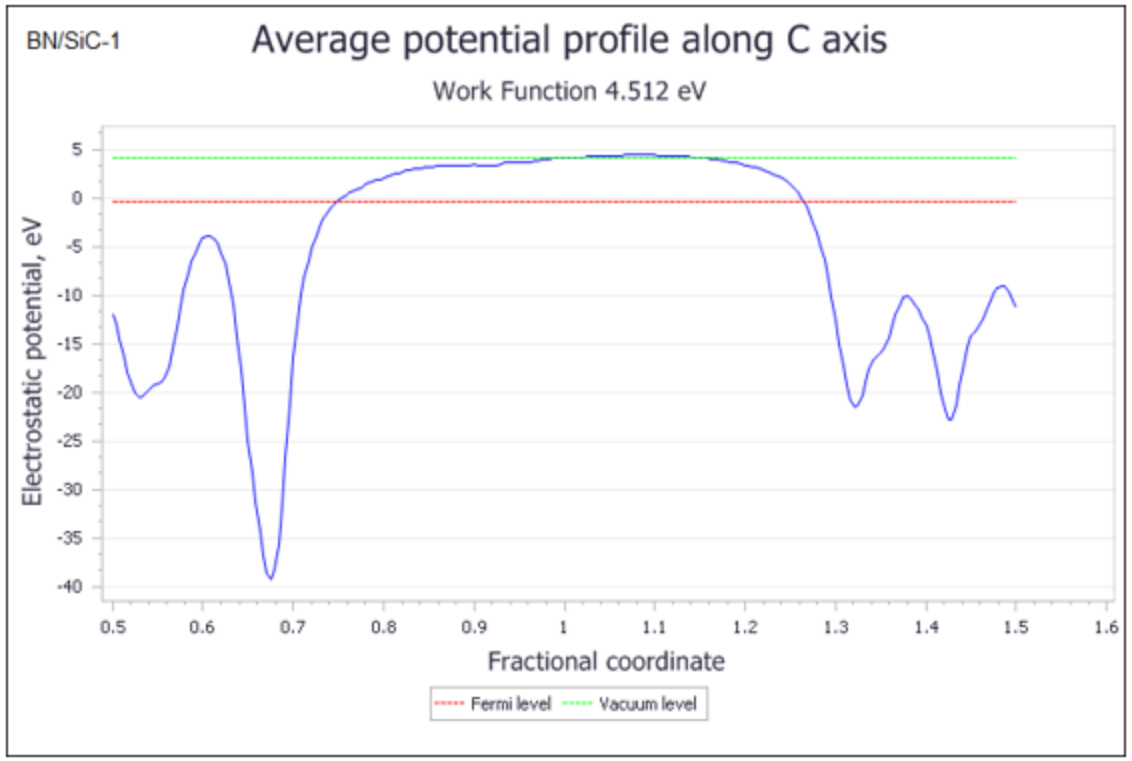
1. The band gaps of BN calculated by Y. R. Tang and J. X. Cao, as is shown in the Fig.1. We calculated band gap(HSE06) of BN is 4.6 eV. The formation energy calculated by Y. R. Tang and J. X. Cao, as is shown in theTable1. We calculated formation energy of BN is 60 meV. (Ref: Y.R. Tang, Y. Zhang, J.X. Cao, J. Appl. Phys., 119 (2016) 195303.)

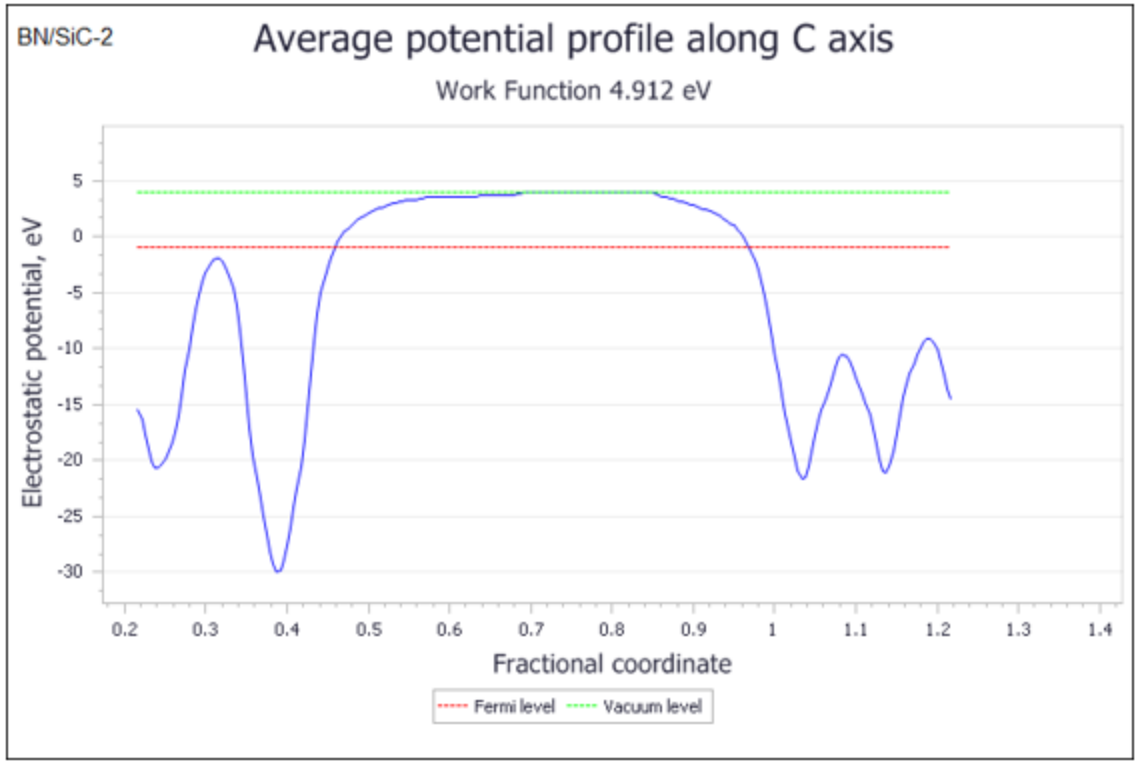


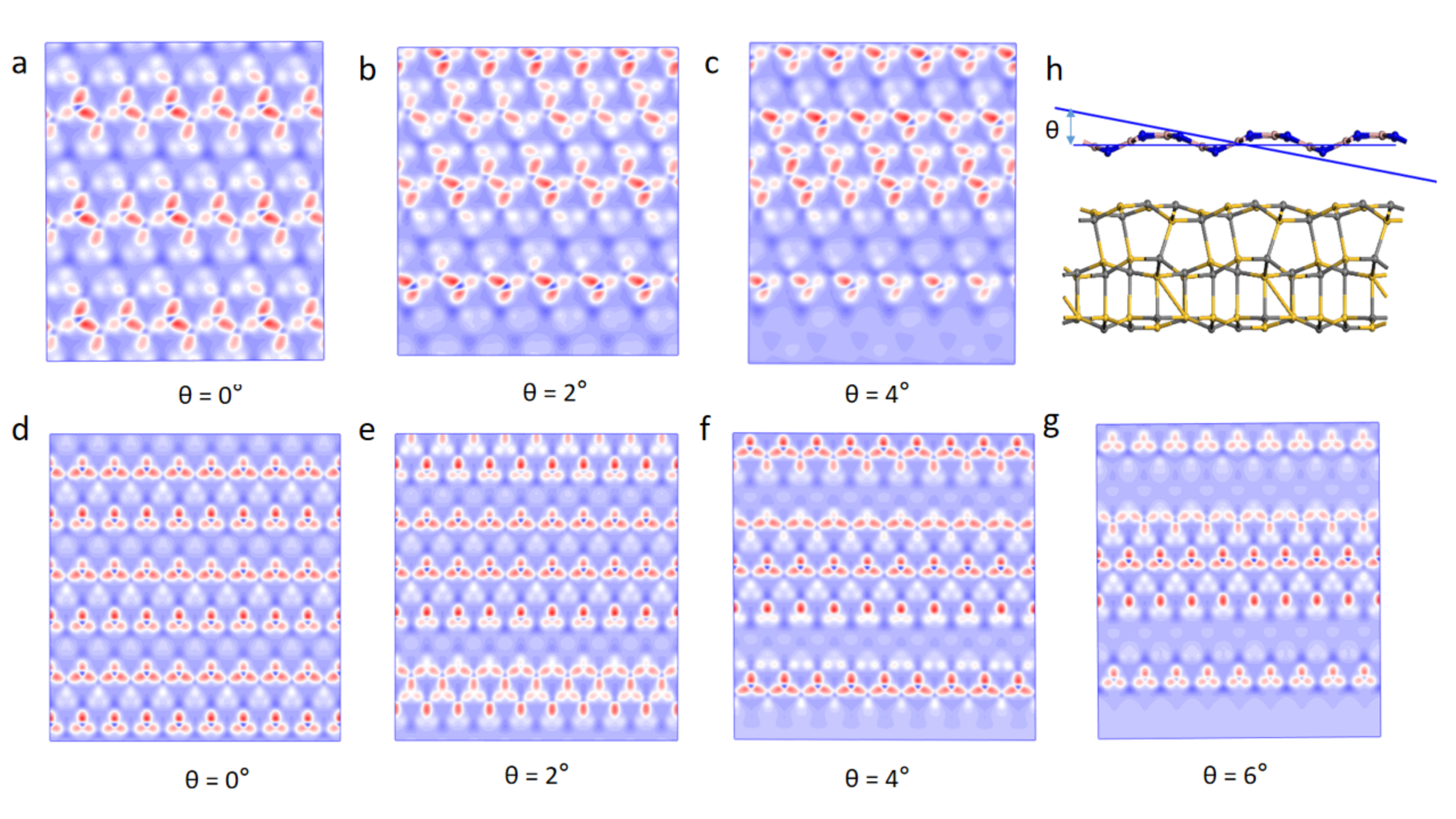
2. Two-dimesional maps for (a) absolute value of the displacement vector u-(r), (b) the local binding energy V [δ(r)]. and (c) strain-induced pseudo magnetic field Beff(r), calculated for Twisted bilayer graphene with various rotation angles. (Ref: Nam N N T, Koshino M. Lattice relaxation and energy band modulation in twisted bilayer graphene[J]. Physical Review B, 2017, 96(7): 075311.)


$\gamma(-\infty)$
$\gamma(1)$
$\gamma(>1)$
$\gamma(1)$
$\gamma(-\infty)$
Barrier
Well
Barrier
$Vcry(r)$ >0
Antibonding
$Vcry(r,B)$
Nonbonding
E_b
$Vcry(r)$ <0
Bonding
E_i

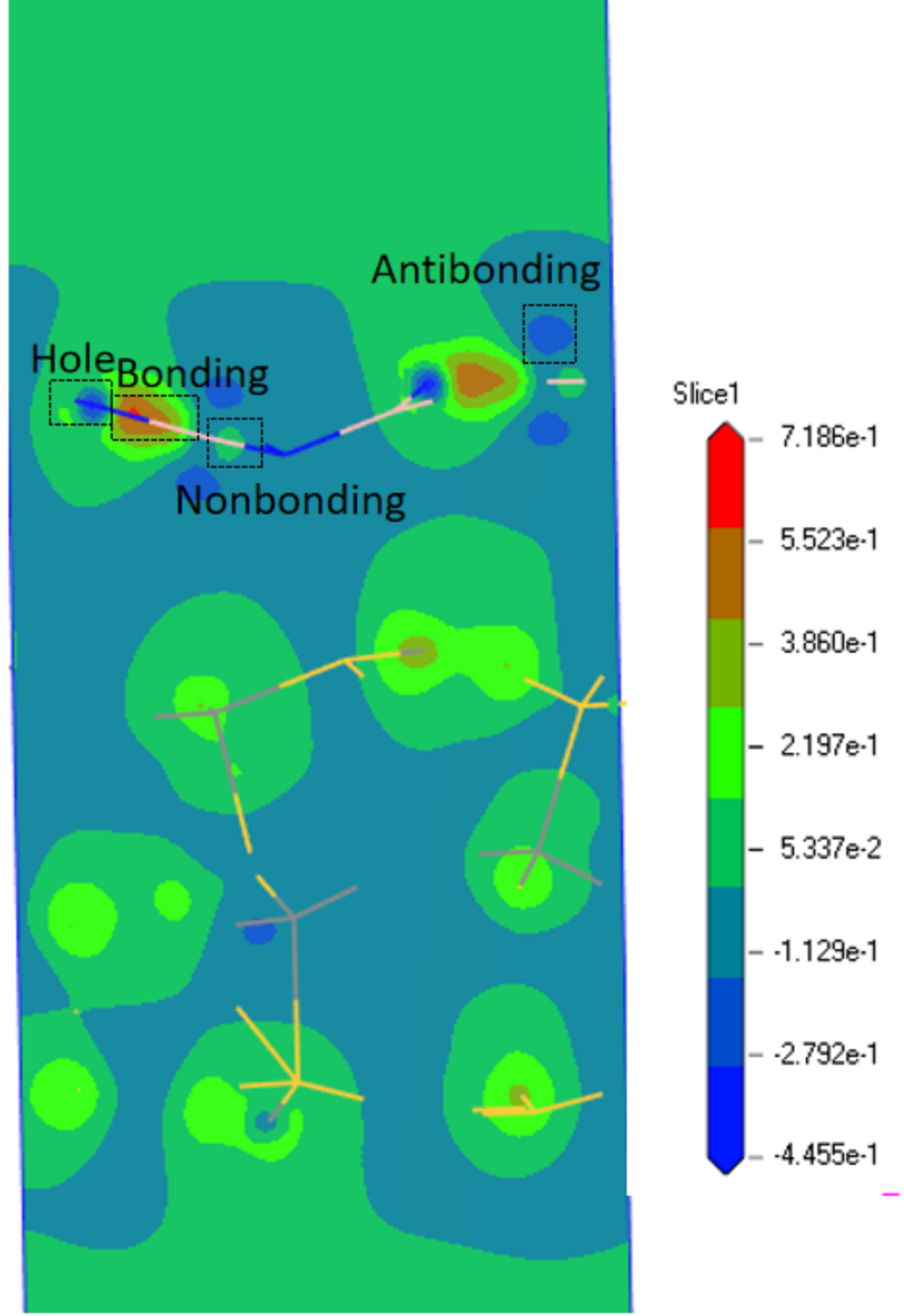

a
b
c
d
Si
B
N
C
1
2
d_{12}
h
h_1


BN/SiC-1
Average potential profile along C axis
Work Function 4.512 eV
Electrostatic potential, eV
5
0
-5
-10
-15
-20
-25
-30
-35
-40
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2
1.3
1.4
1.5
1.6
Fractional coordinate
Fermi level
Vacuum level

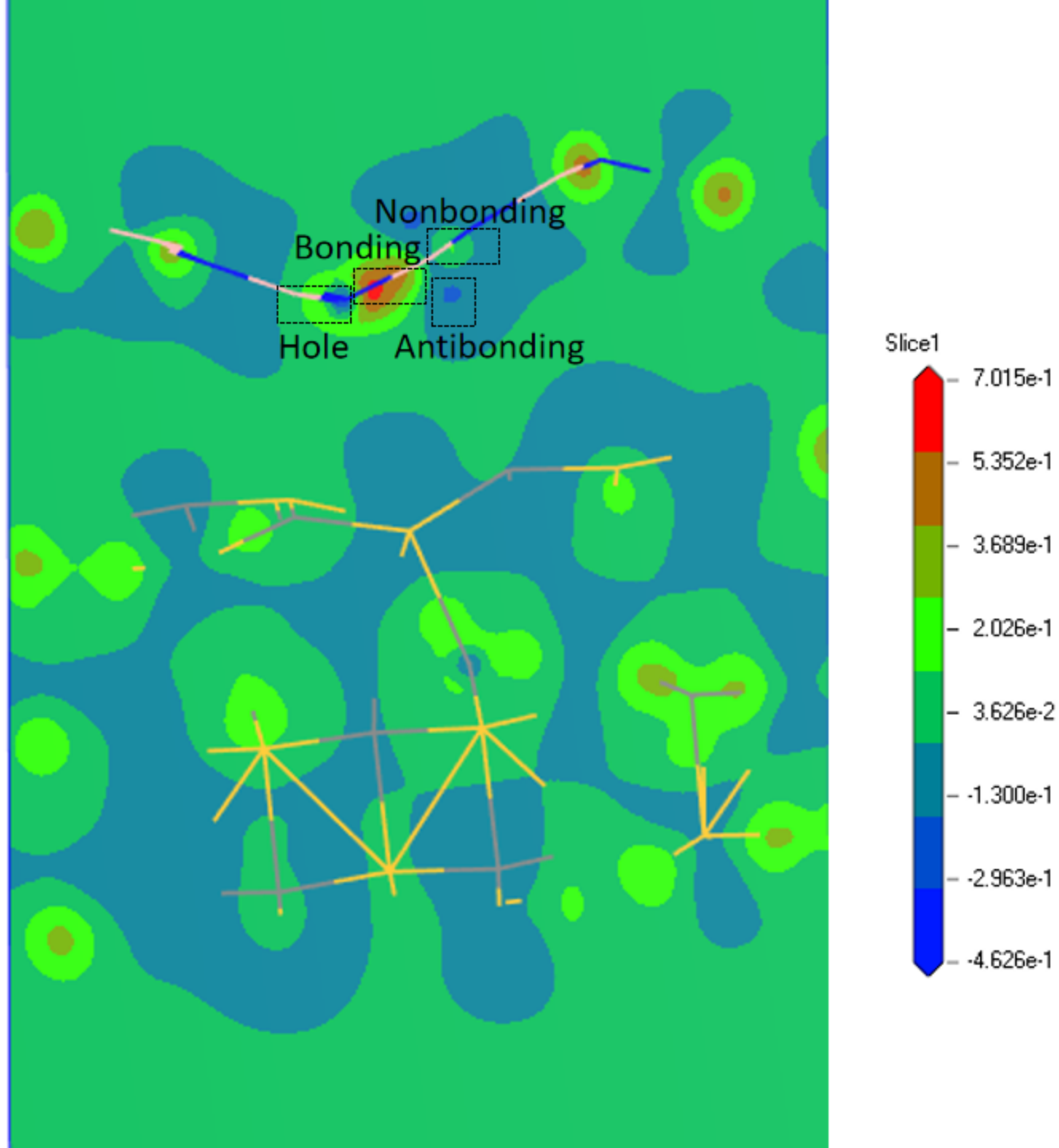

BN/SiC-2
Average potential profile along C axis
Work Function 4.912 eV
Electrostatic potential, eV
5
0
-5
-10
-15
-20
-25
-30
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2
1.3
1.4
Fractional coordinate
Fermi level
Vacuum level


a
b
c
h
θ
θ = 0°
θ = 2°
θ = 4°
d
e
f
g
θ = 0°
θ = 2°
θ = 4°
θ = 6°

a


Antibonding
Hole
Bonding
Nonbonding
Slice1
7.186e-1
5.523e-1
3.860e-1
2.197e-1
5.337e-2
-1.129e-1
-2.792e-1
-4.455e-1

b


Nonbonding
Bonding
Hole
Antibonding
Slice1
7.015e-1
5.352e-1
3.689e-1
2.026e-1
3.626e-2
-1.300e-1
-2.963e-1
-4.626e-1