Cross-Disciplinary Science Forum

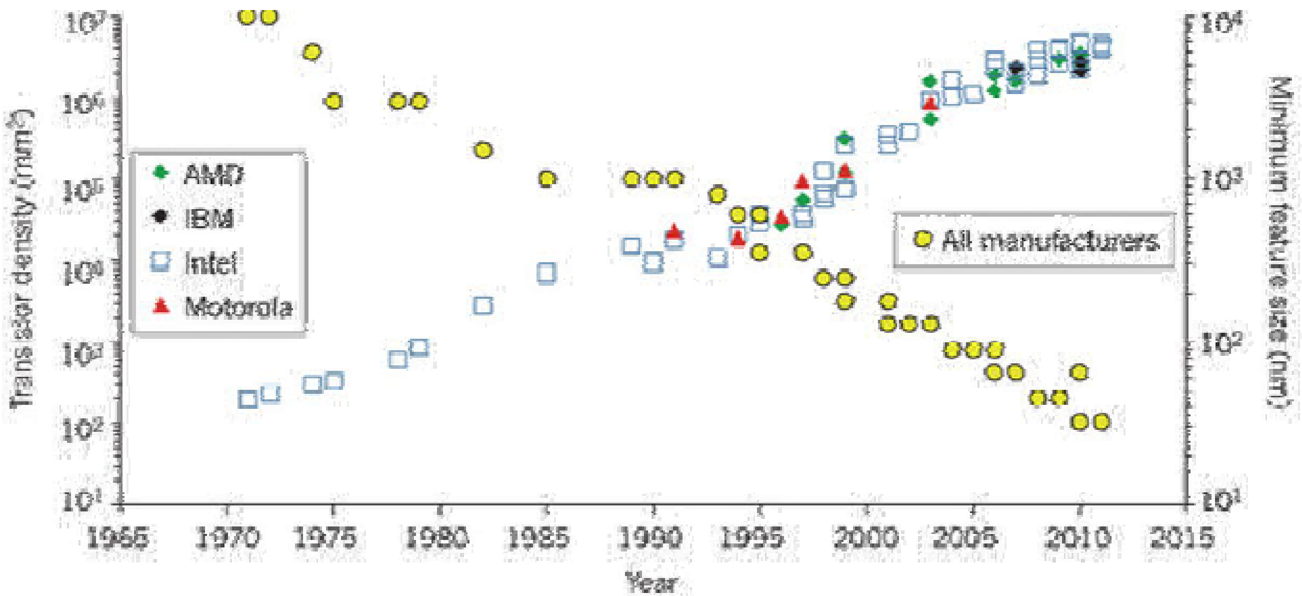
二維的石墨烯半導體

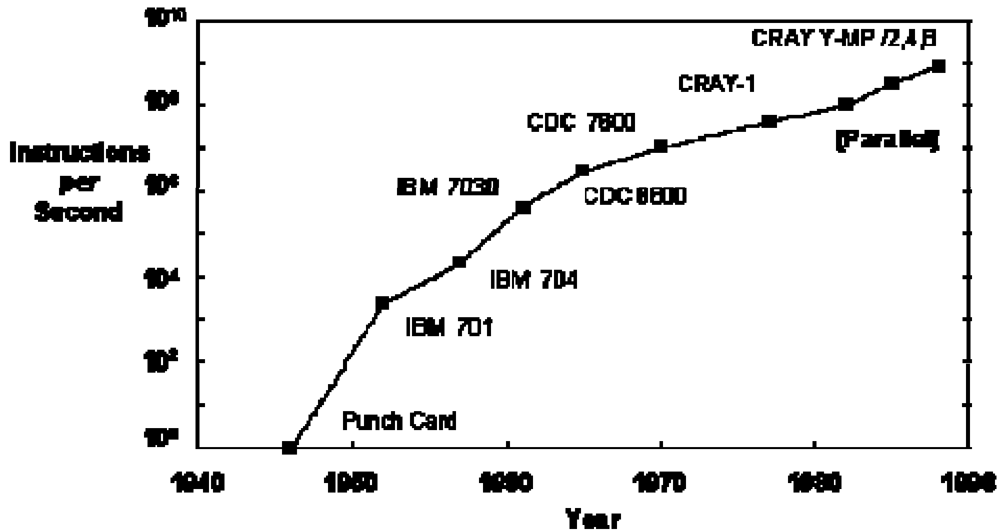
褚志彪

中研院原分所

Moore's Law:

the number of components in integrated circuits had doubled every year from the invention of the integrated circuit in 1958 until 1965 and predicted that the trend would continue "for at least ten years





The Nobel Prize in Physics 2010

Andre Geim, Konstantin Novoselov

Photo: U. Montan

Andre Geim

Photo: U. Montan

Konstantin Novoselov

The Nobel Prize in Physics 2010 was awarded jointly to Andre Geim and Konstantin Novoselov *"for groundbreaking experiments regarding the two-dimensional material graphene"*

石墨烯的特性

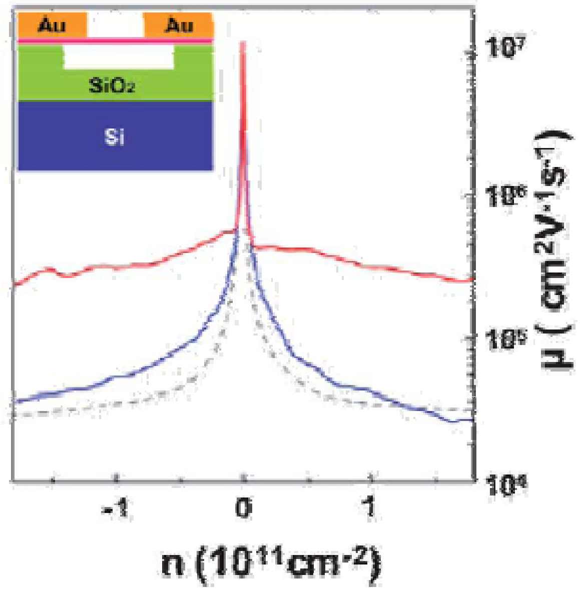
High mobility： > 200000 cm^2/Vs

InSb 77000 cm^2/Vs
Si 1400 cm^2/Vs

$$\frac{1}{\mu_{EFF}} = \frac{1}{\mu_n} + \frac{1}{\mu_{Bal}}$$

$\mu_n \propto \lambda$ mean free path

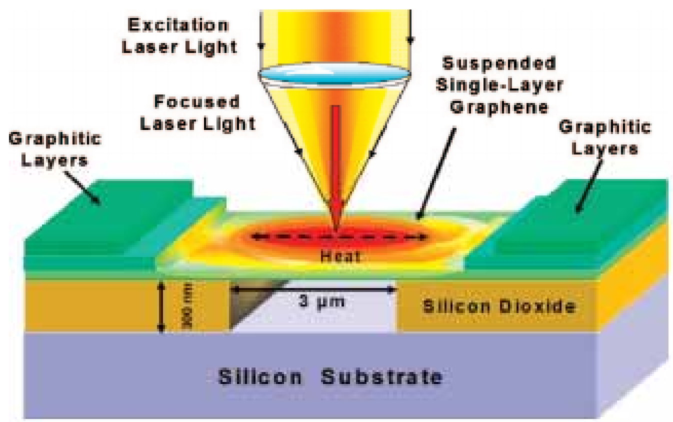
$\mu_{Bal} \propto L$ Device length



Bolotin et al *Solid State Communications* **146** 351 (2008)

Ultra high mobility is not necessary in scaled graphene device

Superior Thermal Conductivity:
~ 5 × 10^3W/mK
dissipate heat quickly, small thermal vibration Effect
Si: 0.7 ~ 3 $Wm^{-1}K^{-1}$



Balandin et al *Nano Letters* **8** 902 (2008)

Low Electric Resistivity:

ρ= 1.0 $\mu\Omega$·cm

銅: 1.72 $\mu\Omega$·cm

Extreme Tensile strength:

~130 G pascals

$$A \geq \frac{W_{大象}}{T_{石墨烯}} = \frac{7000\text{Kg} \times 10\,\frac{m}{s^2}}{130 \times 10^9\,\frac{N}{m^2}} \approx 0.5mm^2$$

Flexibility:

Single-atom-thick sheets, minimum device size.

Ambipolar Electric field effect:

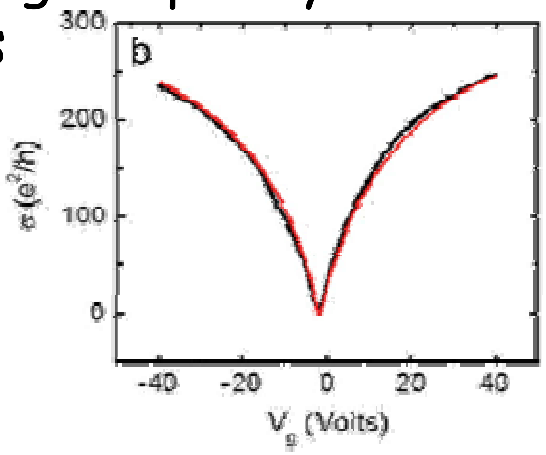
Charge carriers can be tuned continuously between electrons and holes.

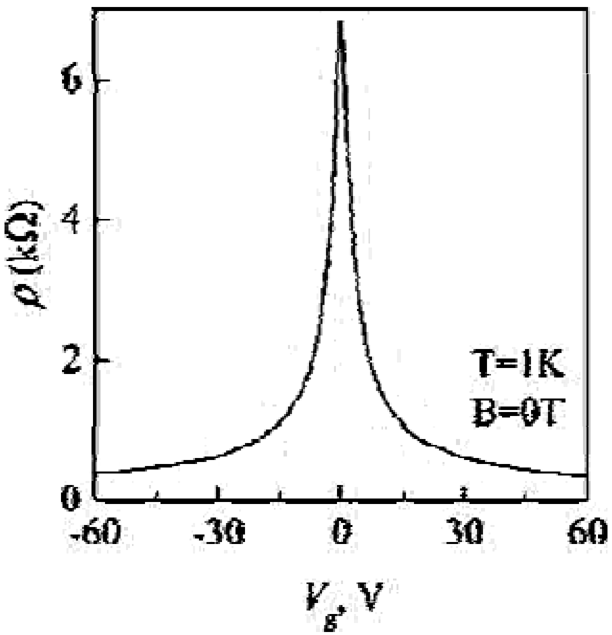
Minimum quantized conductivity:

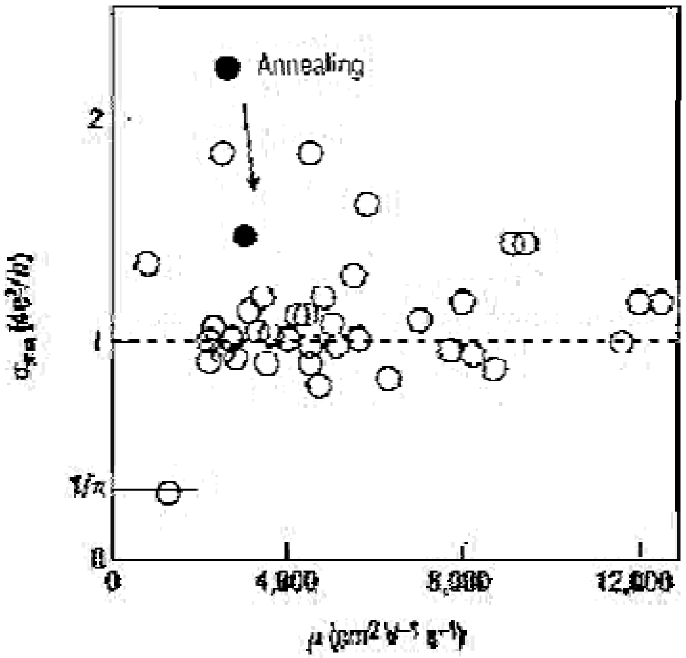
$4e^2/h$ @ **E-field =0**

Due to electron-hole puddles (carrier-density inhomogeneities)

Originated from charge impurity or surface corrugations





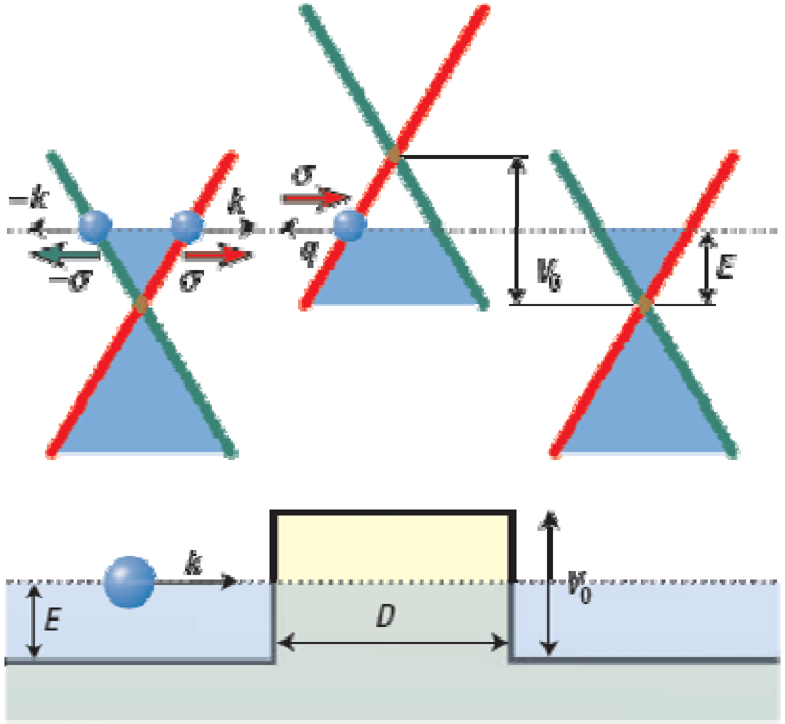


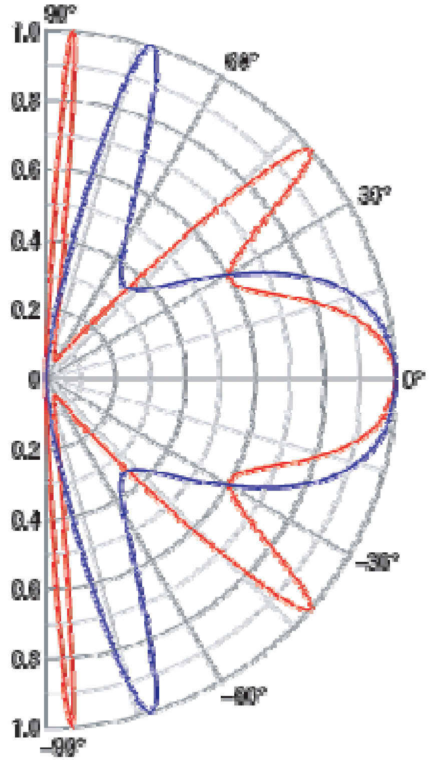
A. K. Geim & K. S. Novoselov
Nature Materials **6**, 183 (2007)

Klein tunneling:

Conservation of Pseudospin. (pseudospin flipping is prohibited)

Weak electrostatic confinement.

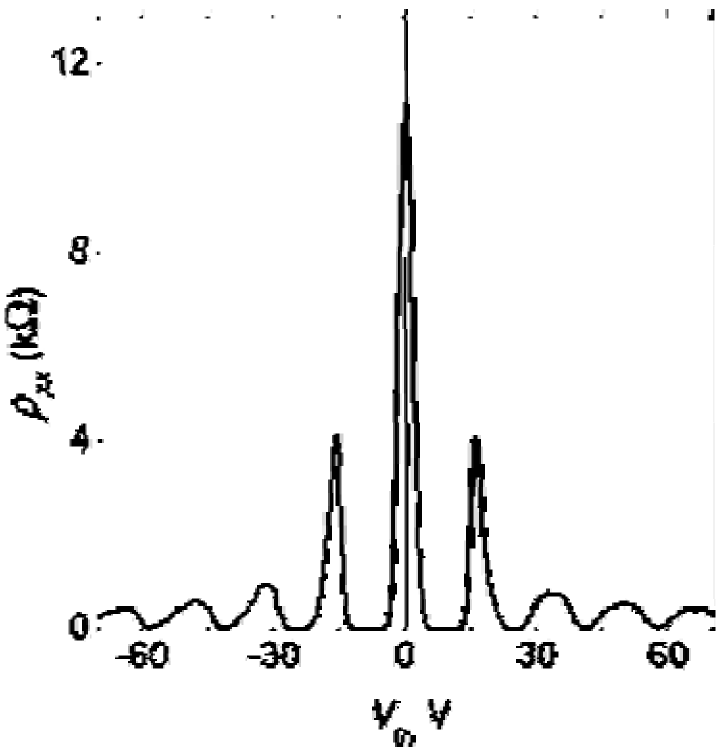


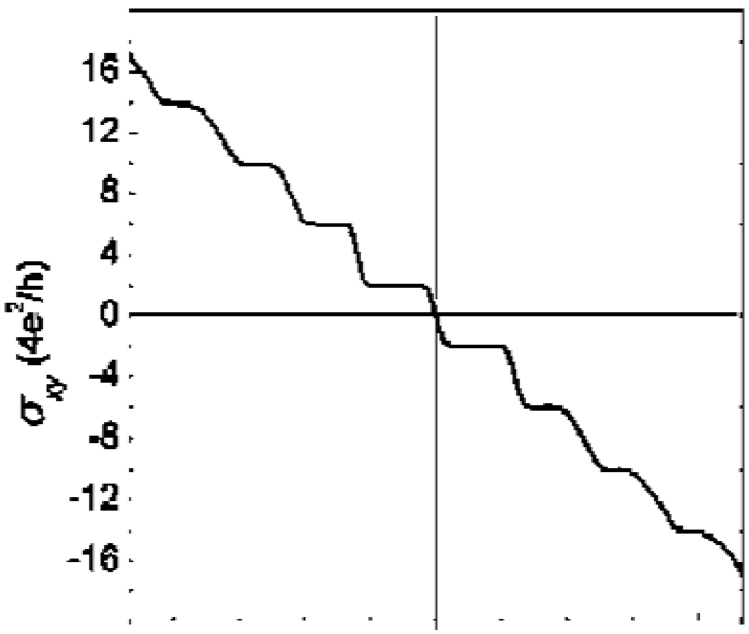


M. Katsnelson et al *Nature Physics 2*, 620 (2006)

Quantum Hall effect:

T=4K; B=14T





K. Novoselov et al phys. Stat. sol. **244**, 4106 (2007)

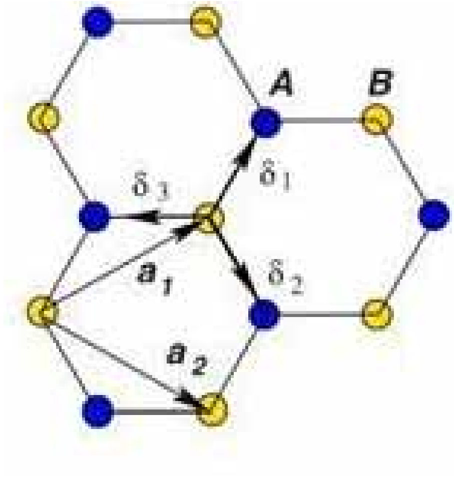
$$\sigma_{xy} = \pm 4e^2/h(N + 1/2)$$

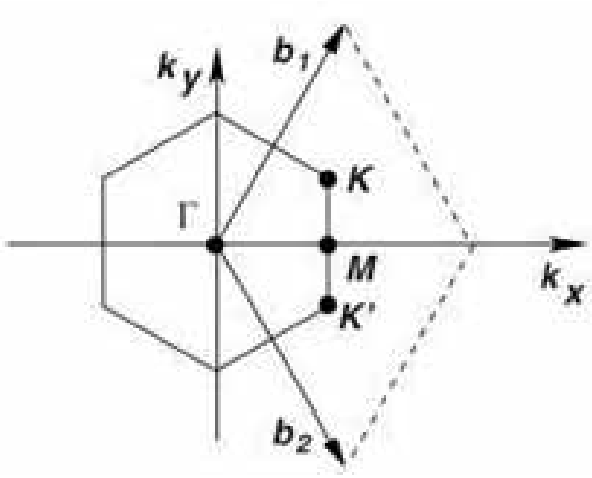
N: Landau Level

↑

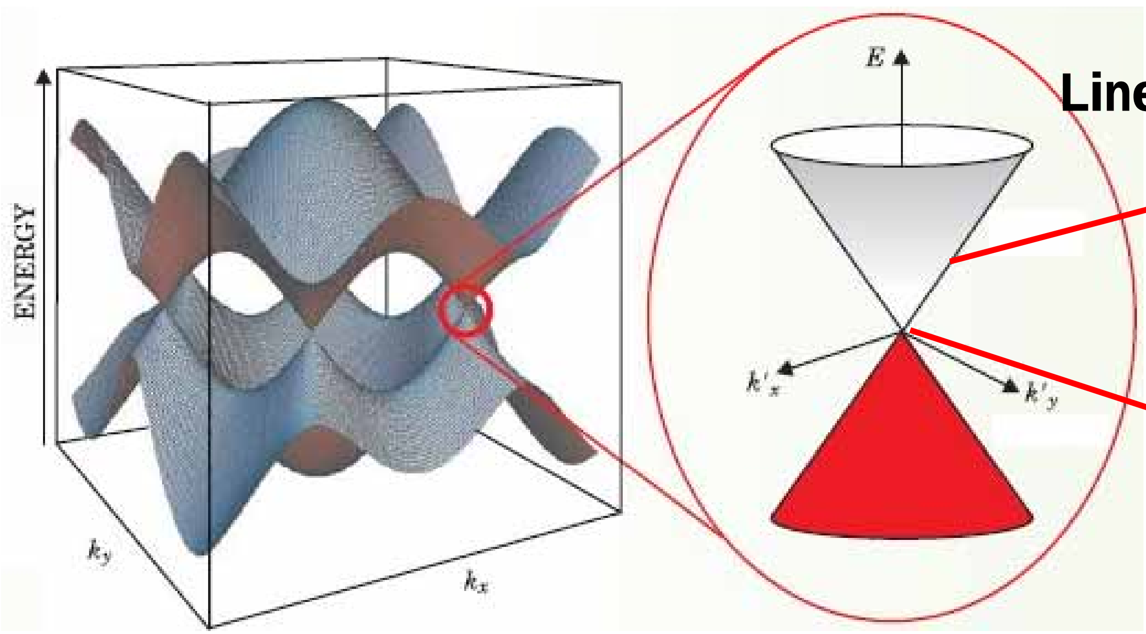
4=2(valley degeneracy)x2(spin degeneracy)

石墨烯的晶格結構





A/B sublattice **K/K' obey space inversion symmetry**

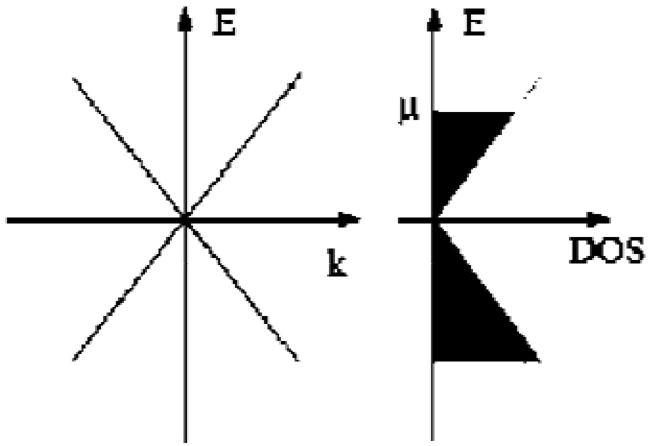


Linear dispersion nearby Dirac point

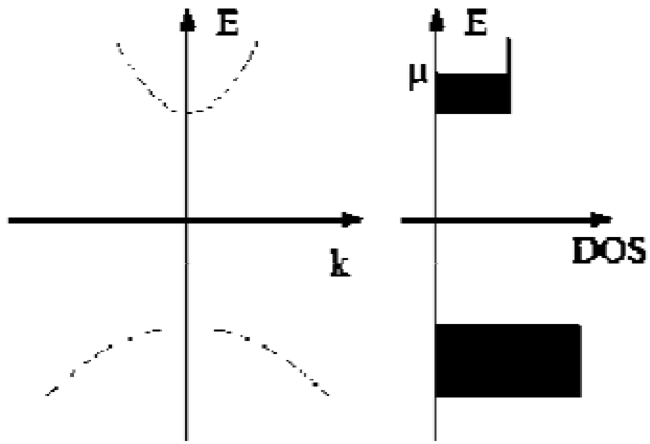
Zero bandgap semiconductor

Electronic Properties

Graphene



2DEG



- $\varepsilon(k)=\pm\hbar v_F k$, no gap
- DOS(E)~E

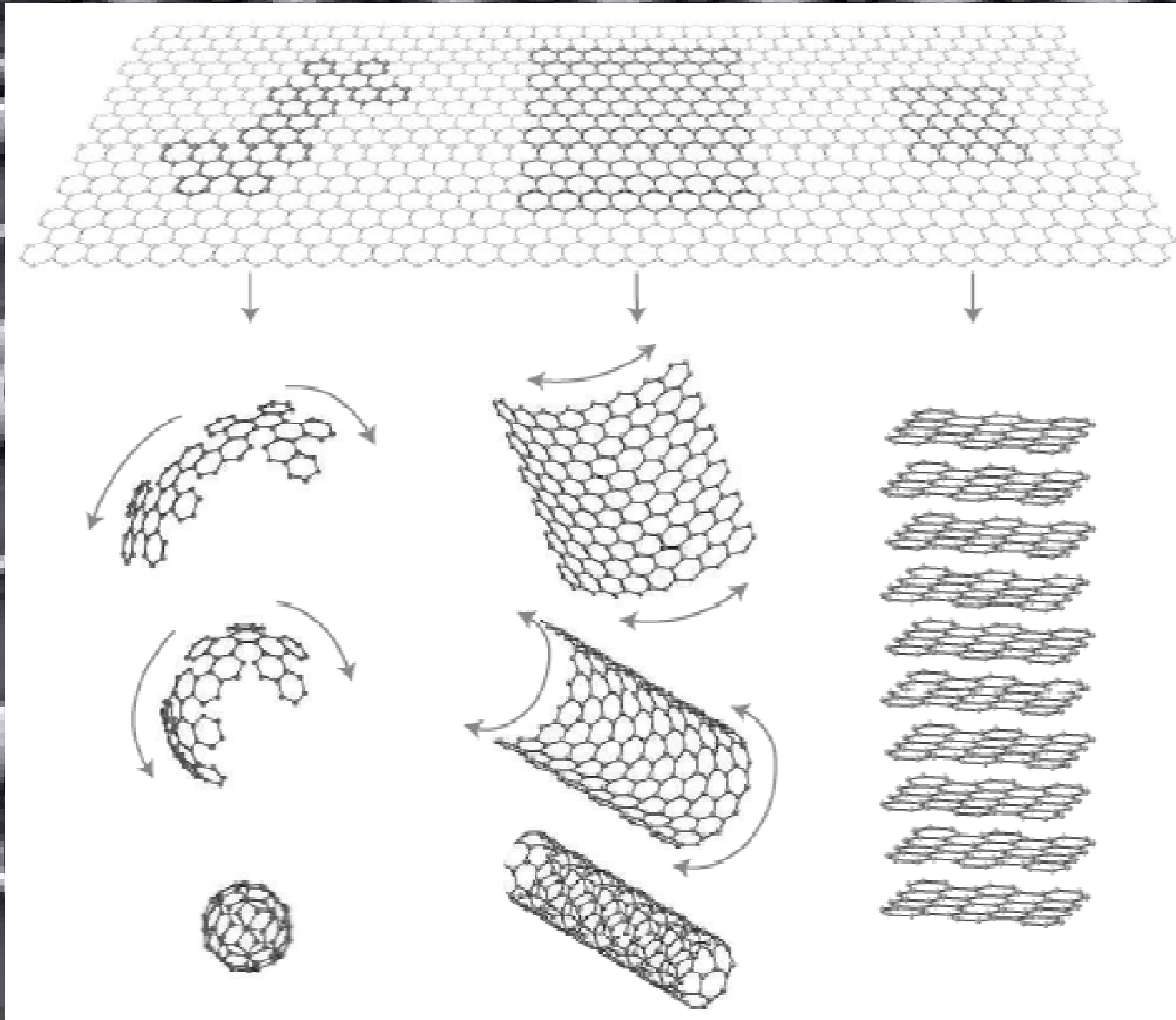
- $\varepsilon(k)=\hbar^2k^2/2m^*$
- DOS(E)=const.

Dirac Fermion:

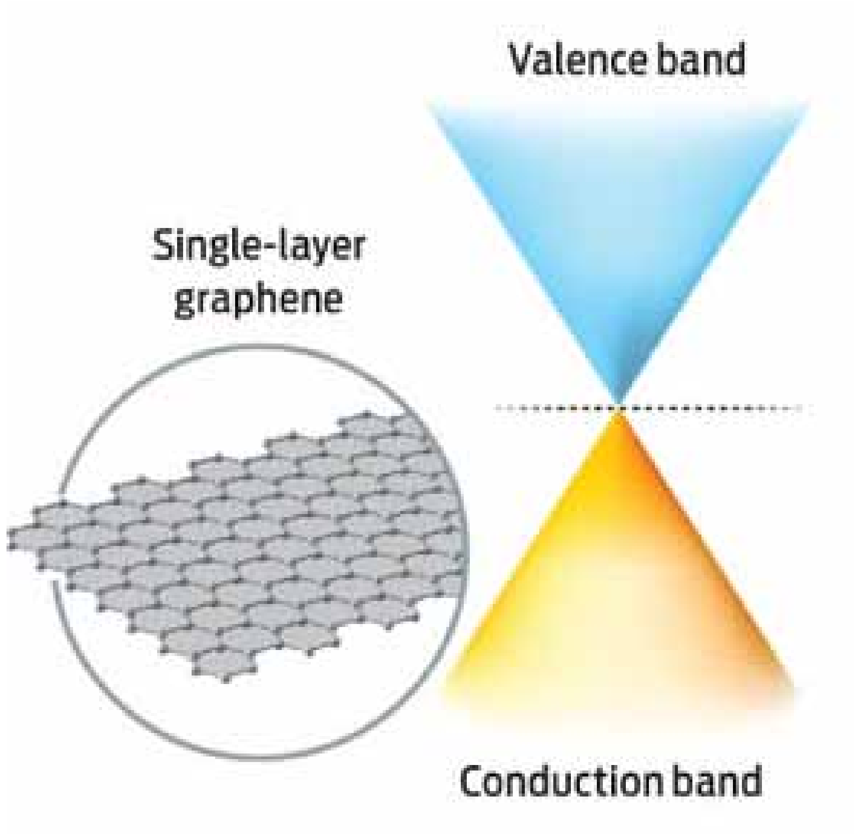
$$E_{Dirac}(k) = \pm\sqrt{\hbar^2c^2k^2 + m^2c^4}$$

$$E_{Gra}(k) = \pm\hbar v_F k$$ $m_{eff}=0$, $v_F \sim 10^6$ m/s

石墨烯的衍生物

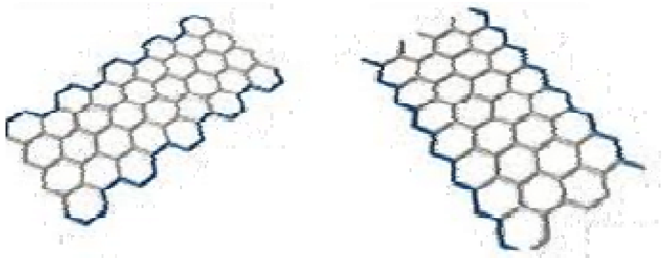


Replacement of Silicon in IC?

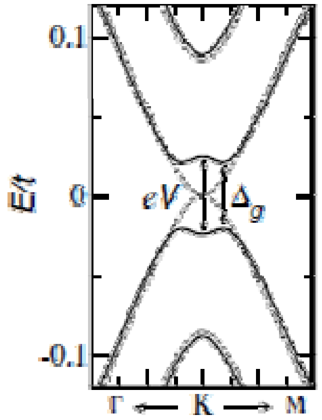


Need a gap (switch on/off) for transistor application.

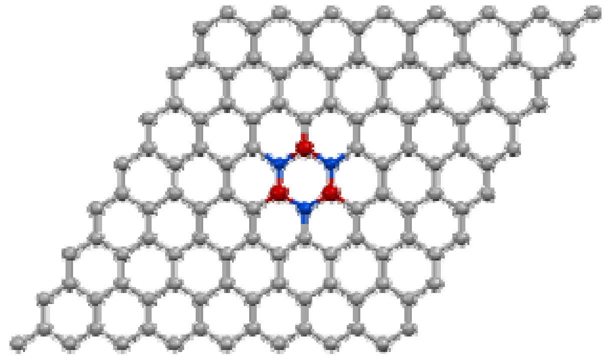
How to open a gap in graphene ?



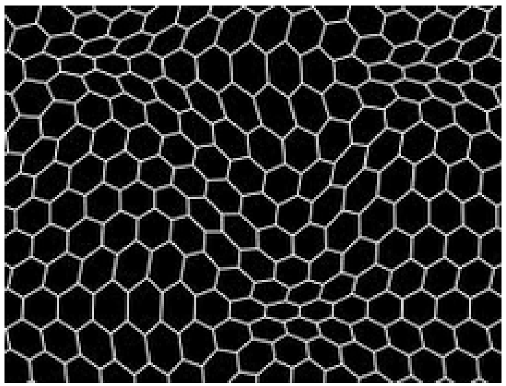
Nnanoribbon



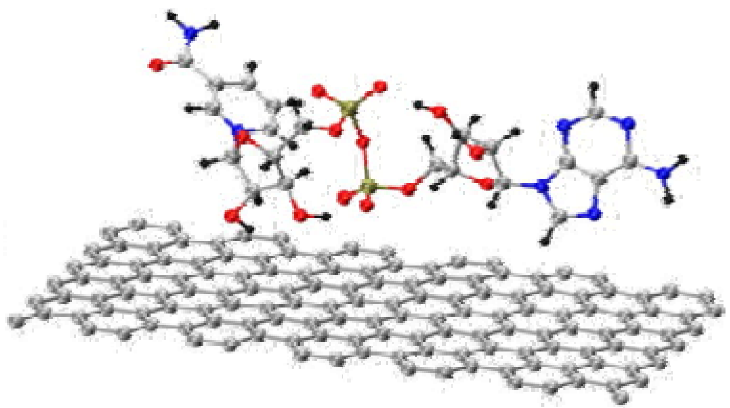
Apply bias on BLG



Chemical substitution

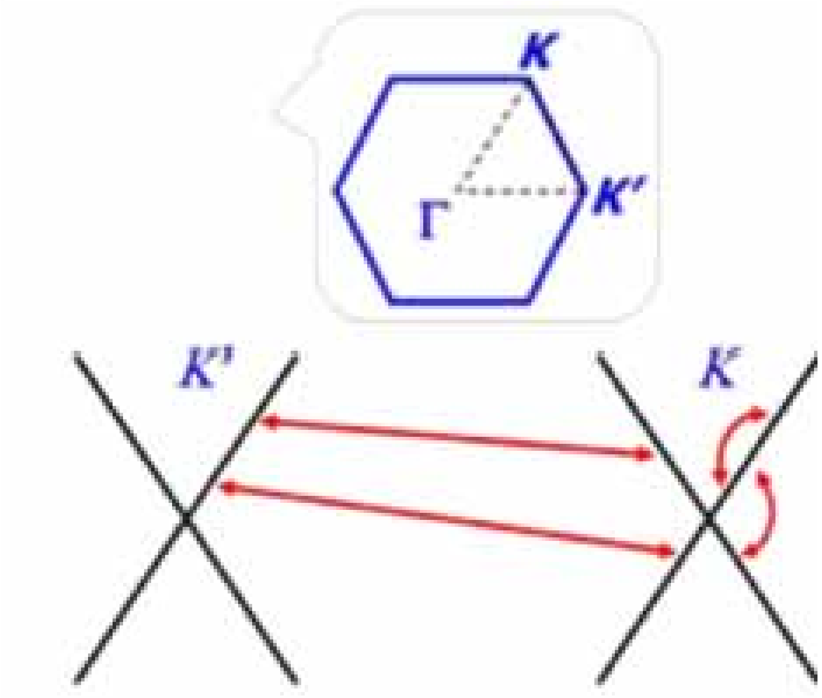


Strain



Molecule absorption

Gap opening mechanism

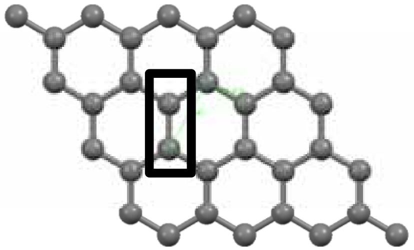


Intra-valley
(sublattice symmetry)

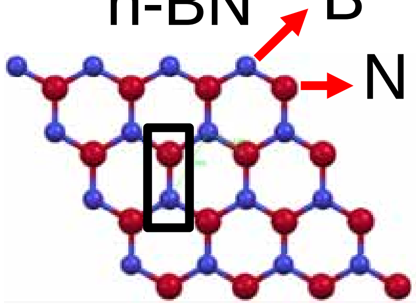
Inter-valley
(chiral symmetry)

Gap opening due to Sublattice symmetry broken

Graphene



h-BN



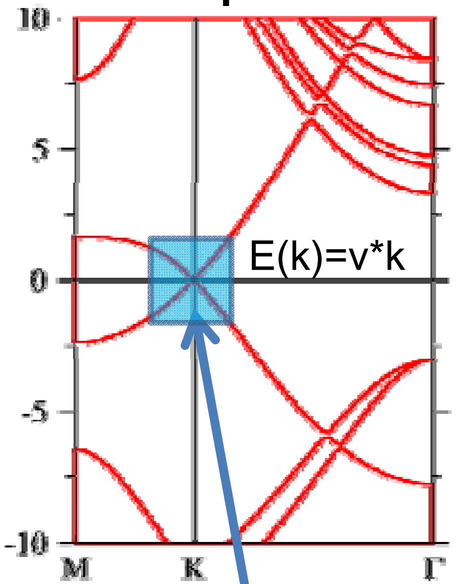
Sublattice Symmetry Broken

Lattice mismatch ~1.7%

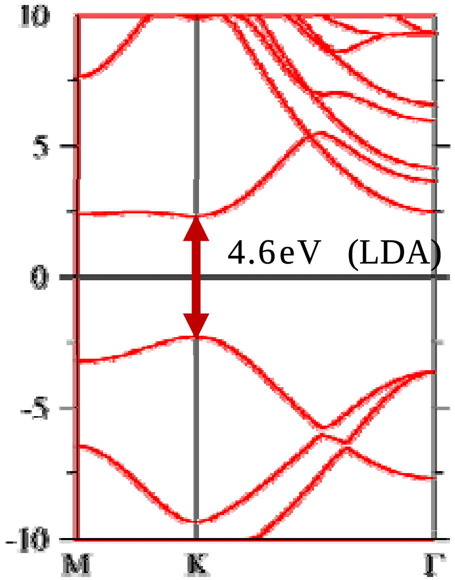
$$\mathbf{E}(\mathbf{k}) = \pm\sqrt{(\mathbf{v}\cdot\mathbf{k})^2 + (E_g/2)^2}$$

On-site energy difference at sublatticies

Graphene



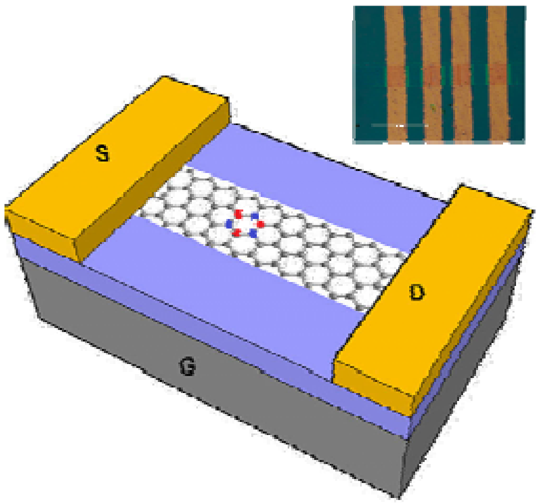
h-BN

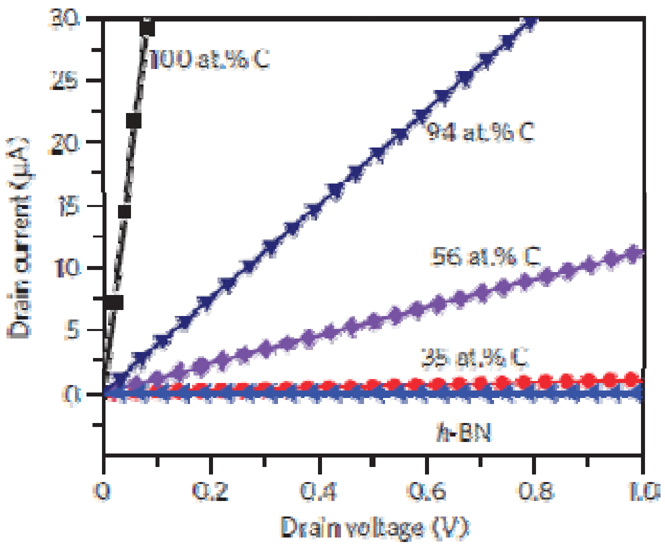


Gapless at
Dirac point

Recent development of h-BNC applications

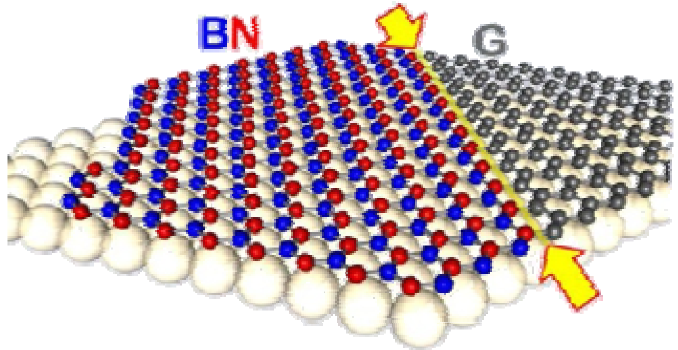
h-BNC FET (2010)





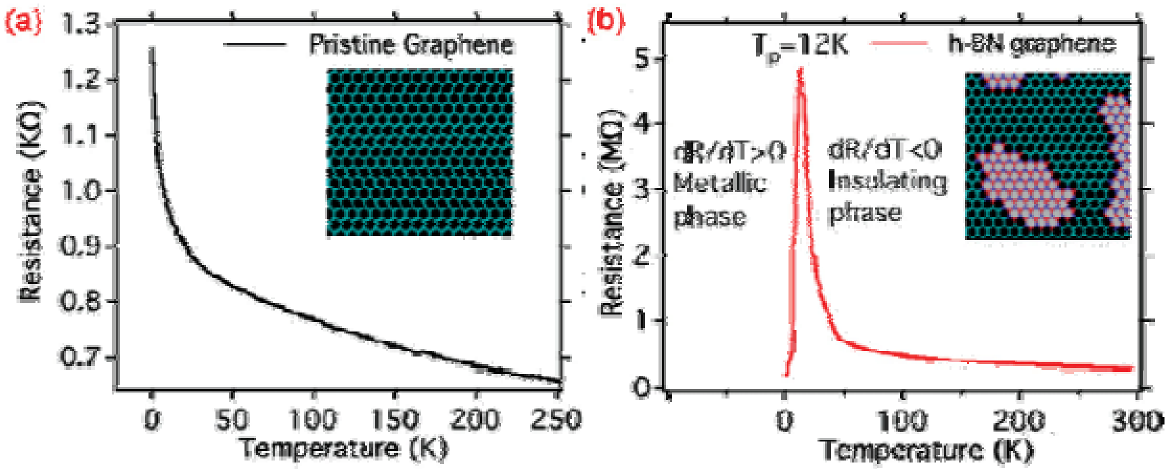
L. Ci et.al. Nature Mat. 2010

Leteral heterostructures



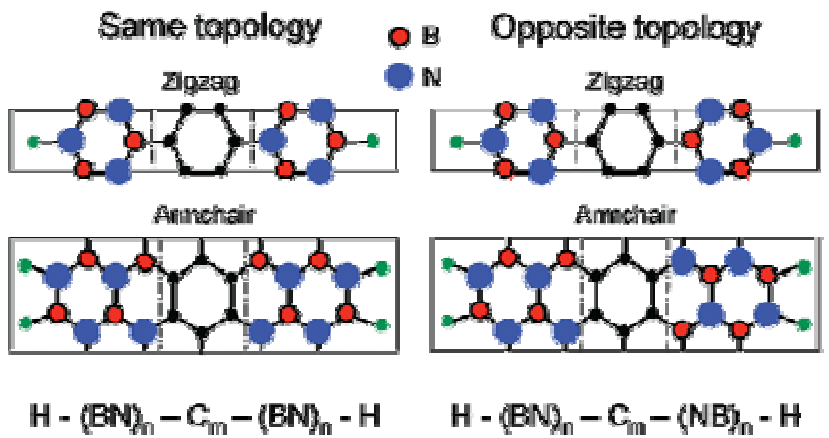
P. Sutter et. al. Nano. Lett. 2012
M. Levendorf et.al. Nature 2012

Anomalous insulator-metal transition (IMT)



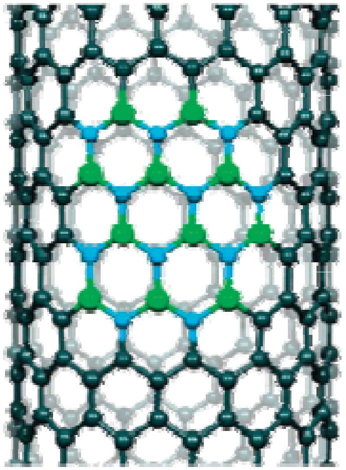
L. Song et.al. Phys. Rev. B 2012

1D transport



J. Jung et.al. Nano Lett. 2012

BN Domains embedded in Carbon Nanotubes



A strong tendency for the formation of BN pairs and, subsequently, BN hexagons within the carbon lattice. At higher doping concentrations, it is found that the formation of compact BN domains would be the most energetically favorable. The importance of a correct description of the BN/C frontier, due to the large border/surface ratio of small dopant domains.

V. Ivanovskaya et.al.J. Phys. Chem. C 2009

Periodic Table of the Elements

Valence

http://chemistry.about.com

Maximum Valence

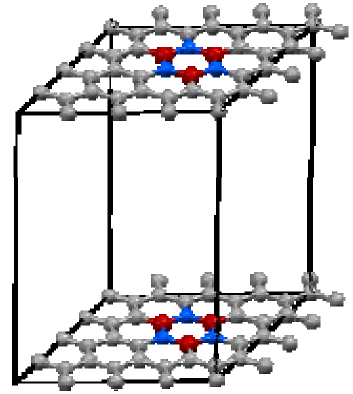
0	1	2	3	4	5	6	7

1A	2A	3B	4B	5B	6B	7B	8B	8B	8B	1B	2B	3A	4A	5A	6A	7A	8A
1 H Hydrogen																	2 He Helium
3 Li Lithium	4 Be Beryllium											5 B Boron	6 C Carbon	7 N Nitrogen	8 O Oxygen	9 F Fluorine	10 Ne Neon
11 Na Sodium	12 Mg Magnesium											13 Al Aluminum	14 Si Silicon	15 P Phosphorus	16 S Sulfur	17 Cl Chlorine	18 Ar Argon
19 K Potassium	20 Ca Calcium	21 Sc Scandium	22 Ti Titanium	23 V Vanadium	24 Cr Chromium	25 Mn Manganese	26 Fe Iron	27 Co Cobalt	28 Ni Nickel	29 Cu Copper	30 Zn Zinc	31 Ga Gallium	32 Ge Germanium	33 As Arsenic	34 Se Selenium	35 Br Bromine	36 Kr Krypton
37 Rb Rubidium	38 Sr Strontium	39 Y Yttrium	40 Zr Zirconium	41 Nb Niobium	42 Mo Molybdenum	43 Tc Technetium	44 Ru Ruthenium	45 Rh Rhodium	46 Pd Palladium	47 Ag Silver	48 Cd Cadmium	49 In Indium	50 Sn Tin	51 Sb Antimony	52 Te Tellurium	53 I Iodine	54 Xe Xenon
55 Cs Cesium	56 Ba Barium	57-71 Lanthanides	72 Hf Hafnium	73 Ta Tantalum	74 W Tungsten	75 Re Rhenium	76 Os Osmium	77 Ir Iridium	78 Pt Platinum	79 Au Gold	80 Hg Mercury	81 Tl Thallium	82 Pb Lead	83 Bi Bismuth	84 Po Polonium	85 At Astatine	86 Rn Radon
87 Fr Francium	88 Ra Radium	89-103 Actinides	104 Rf Rutherfordium	105 Db Dubnium	106 Sg Seaborgium	107 Bh Bohrium	108 Hs Hassium	109 Mt Meitnerium	110 Ds Darmstadtium	111 Rg Roentgenium	112 Cn Copernicium	113 Uut Ununtrium	114 Fl Flerovium				

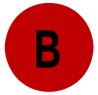
Lanthanides	57 La Lanthanum	58 Ce Cerium	59 Pr Praseodymium	60 Nd Neodymium	61 Pm Promethium	62 Sm Samarium	63 Eu Europium	64 Gd Gadolinium	65 Tb Terbium	66 Dy Dysprosium	67 Ho Holmium	68 Er Erbium	69 Tm Thulium	70 Yb Ytterbium	71 Lu Lutetium
Actinides	89 Ac Actinium	90 Th Thorium	91 Pa Protactinium	92 U Uranium	93 Np Neptunium	94 Pu Plutonium	95 Am Americium	96 Cm Curium	97 Bk Berkelium	98 Cf Californium	99 Es Einsteinium	100 Fm Fermium	101 Md Mendelevium	102 No Nobelium	103 Lr Lawrencium

Gap opening due to Sublattice symmetry broken

1st Principles calculation (PAW-LDA)

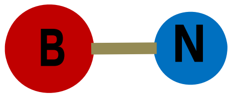


Slab model

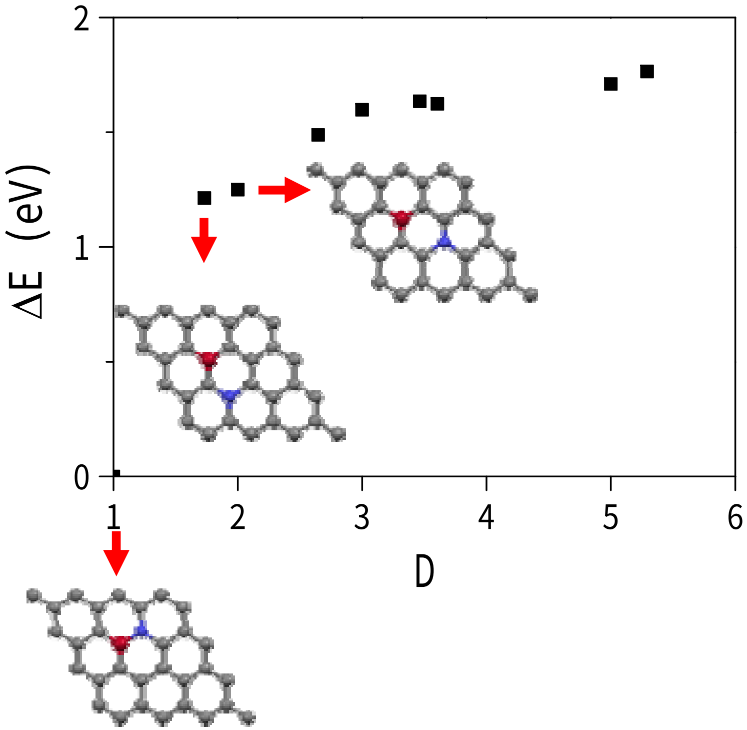


B (one electron less than C): p-dopant

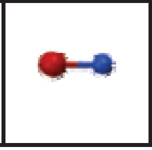
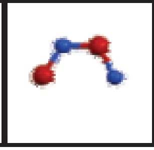
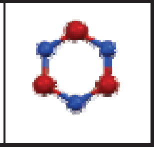
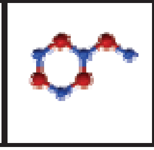
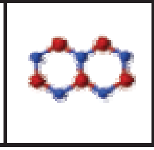
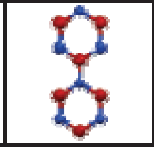
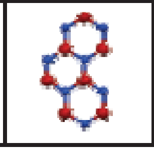
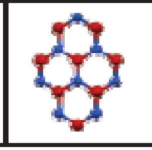
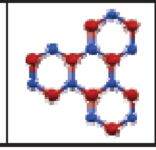
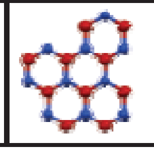
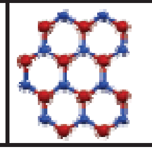
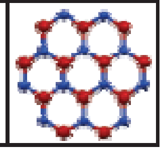
N (one electron less than C): n-dopant



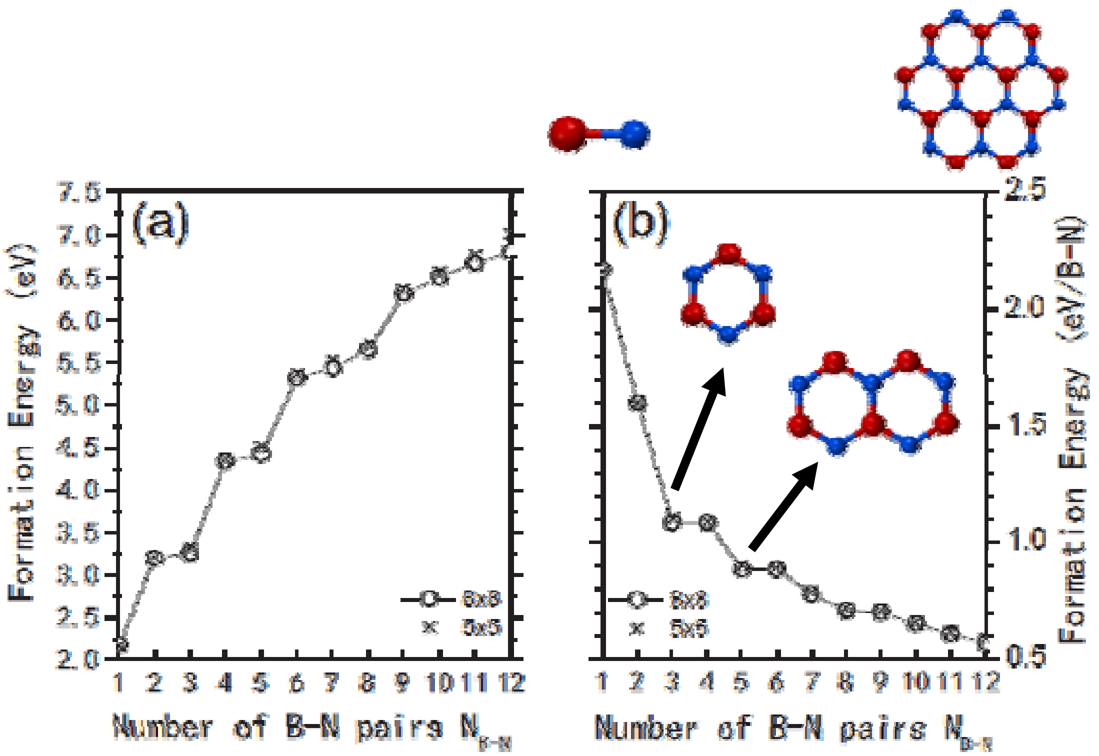
B-N (Effective dipole)

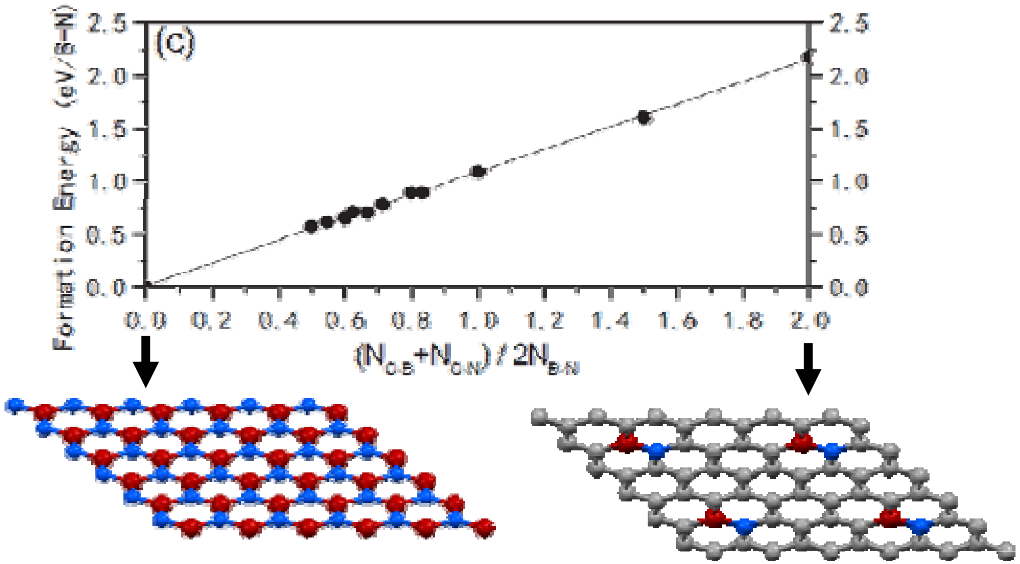


Energetics structures of B-N clusters in h-BNC : Phase Seperation

Optimized structures of B-N dopants on 8 × 8 supercell												
$N_{B\text{-}N}$	1	2	3	4	5	6	7	8	9	10	11	12
$\frac{N_{C\text{-}B}+N_{C\text{-}N}}{2N_{B\text{-}N}}$	2.00	1.50	1.00	1.00	0.80	0.83	0.71	0.63	0.67	0.60	0.55	0.50
Structure												

$$E_{F.E.} = E - N_{B\text{-}N}\mu_{B\text{-}N} - 2(N^2 - N_{B\text{-}N})\mu_C$$



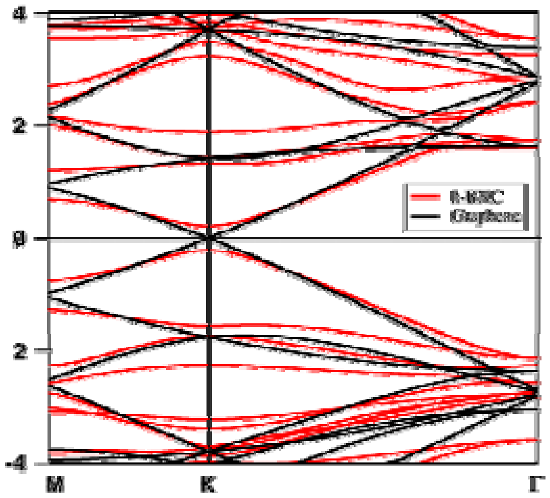


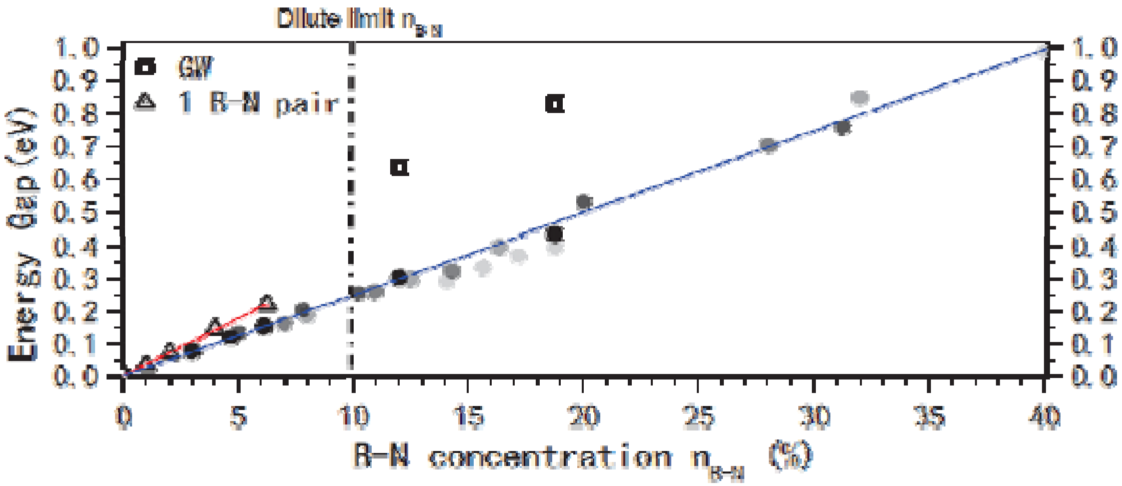
Formation Energy as number of B-N pair of h-BNC

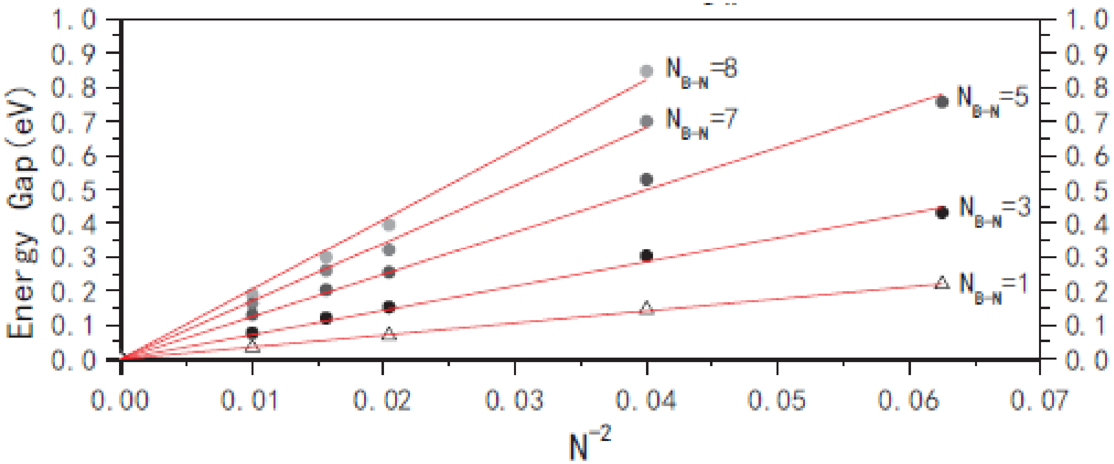
Phase separation is energetic.
C.-P. Chuu et.al. 2012

Gap opening of B-N clusters in h-BNC : Low concentration

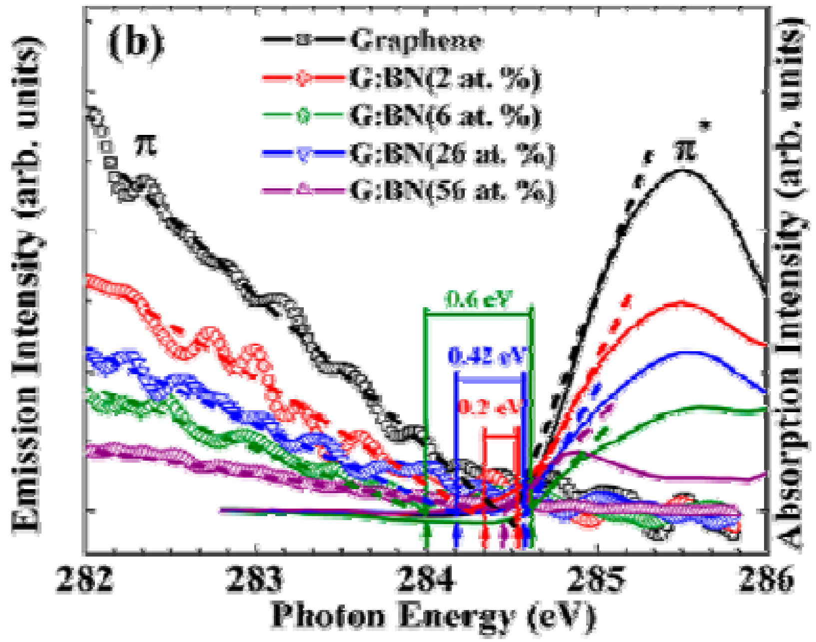
Band Structure of 4x4 h-BNC and pristine graphene



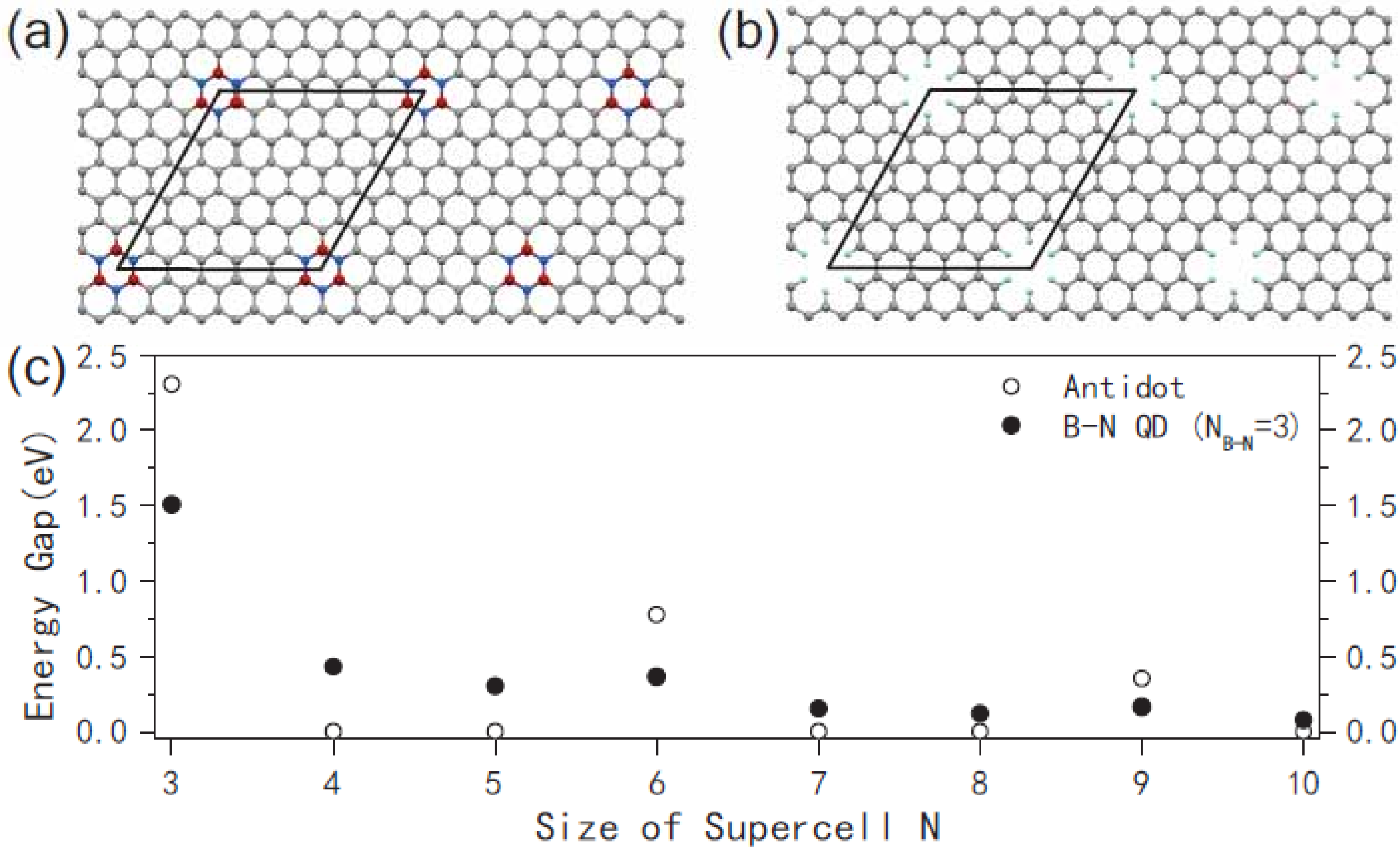




Energy gap vs B-N concentration of h-BNC
C.-P. Chuu et.al. 2012



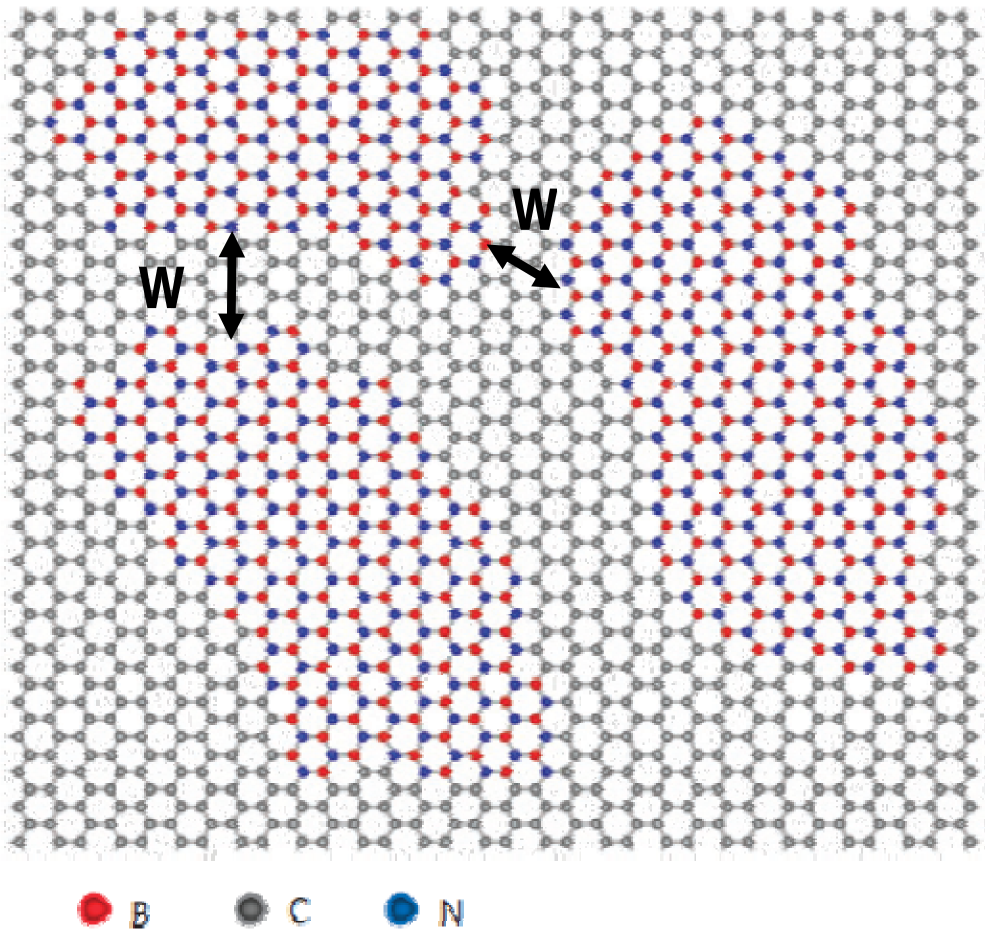
XANES (X-ray Absorption Near-Edge Structure)
C-K Chang et.al. ACS Nano 2013

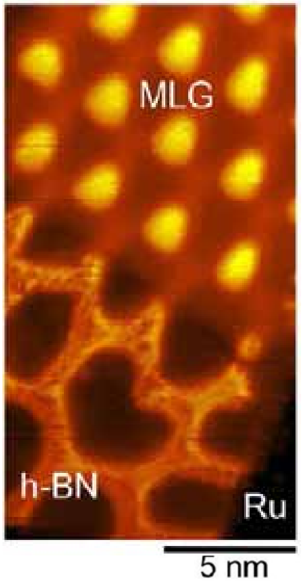


(a)
(b)
(c)
2.5
2.0
1.5
1.0
0.5
0.0
Energy Gap(eV)
Antidot
B-N QD (N_{B-N}=3)
3
4
5
6
7
8
9
10
Size of Supercell N

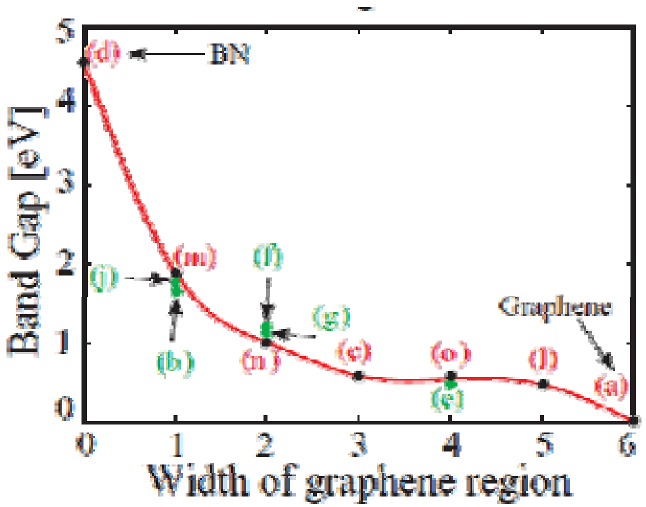
Gap opening of B-N clusters in h-BNC : High concentration

Phase Separation

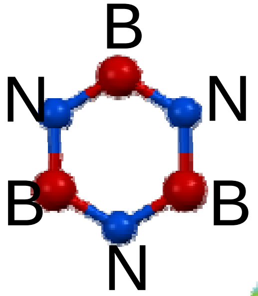




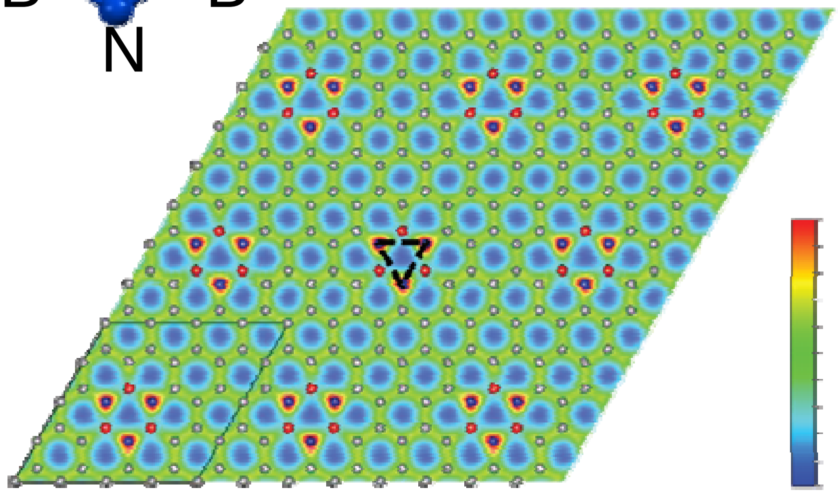
STM
P. Sutter et. al. Nano. Lett. 2011



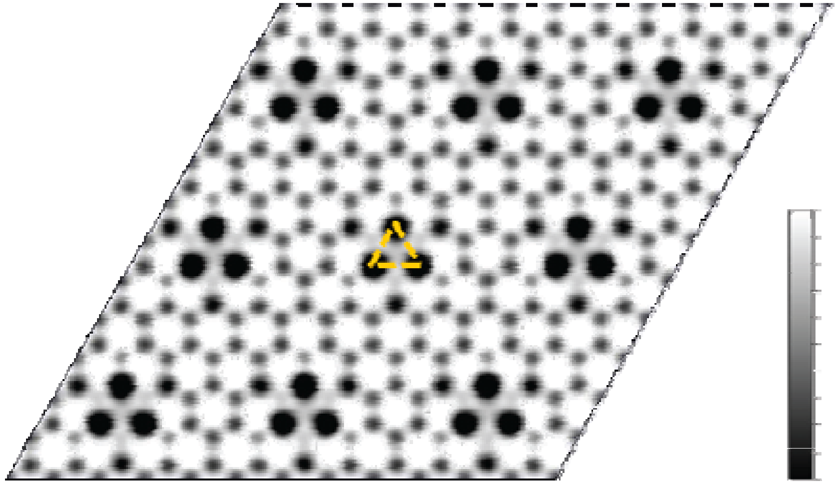
P. Shinde and V. Kumar, Phys. Rev. B 2011



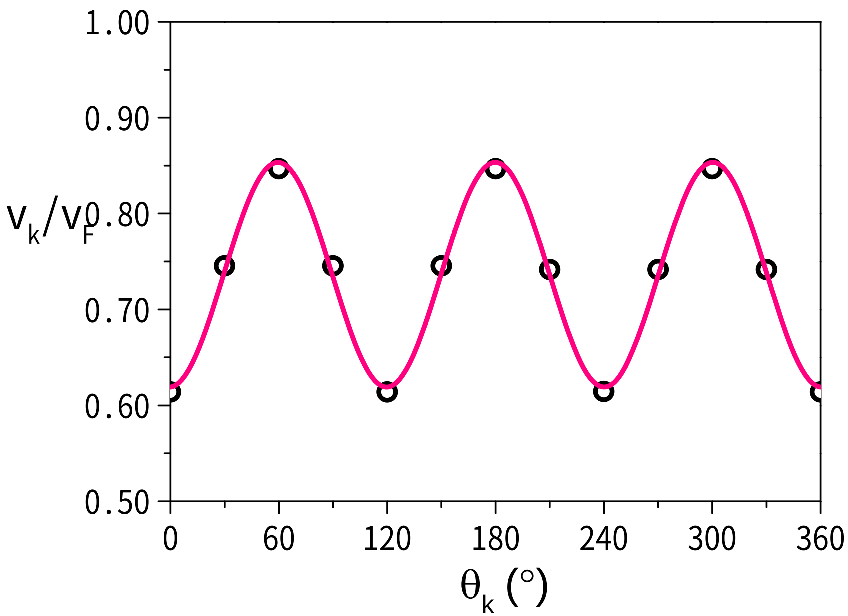
Anisotropy behavior of Dirac fermions in h-BNC

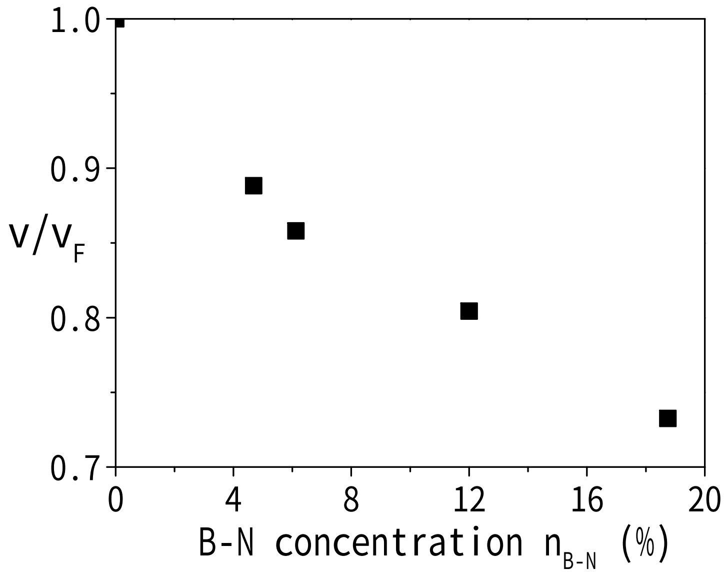


Charge density



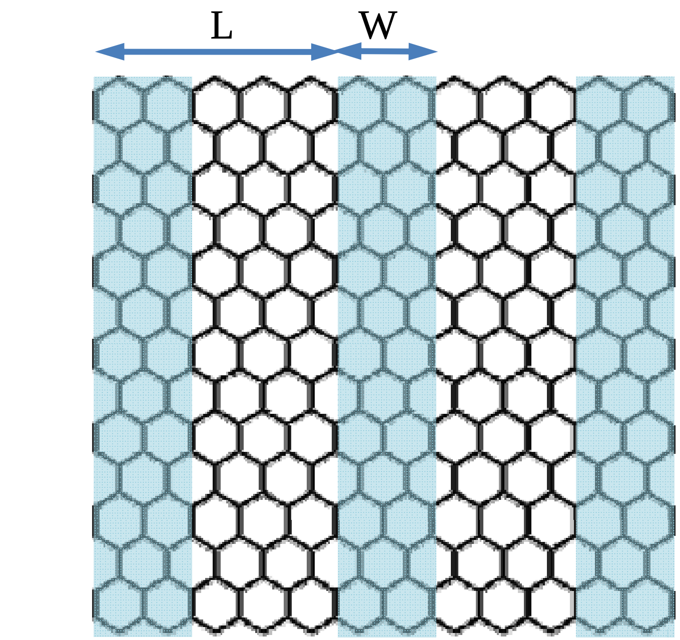
Local potential surface

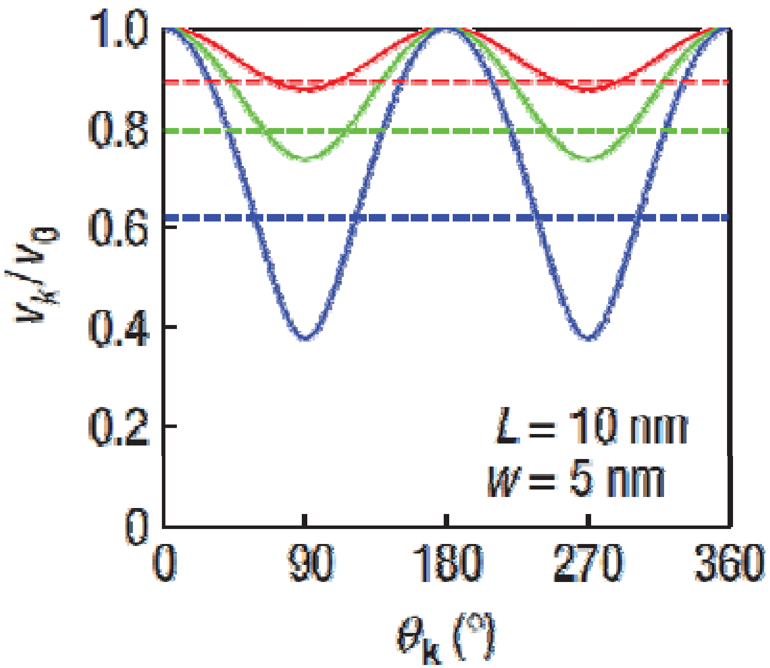


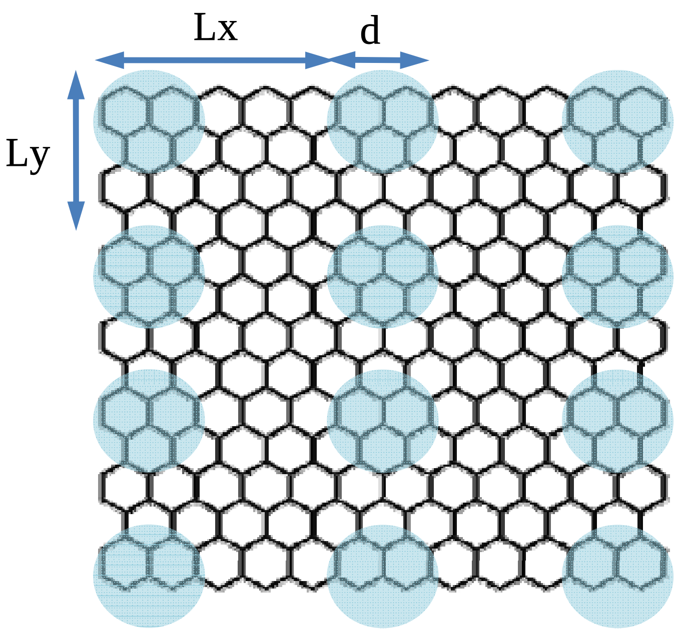


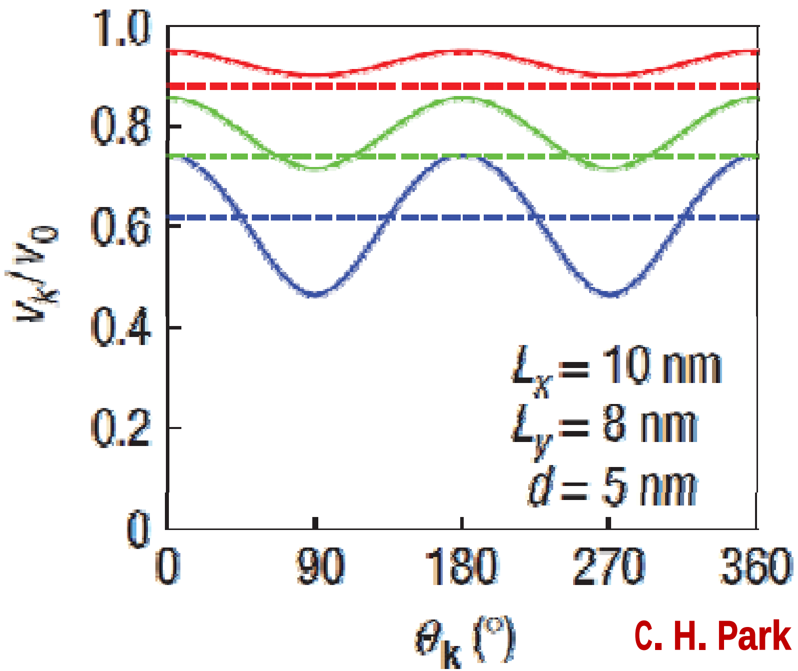
C.-P. Chuu et.al. 2012

Anisotropy behavior of Dirac fermions in graphene under periodic potential



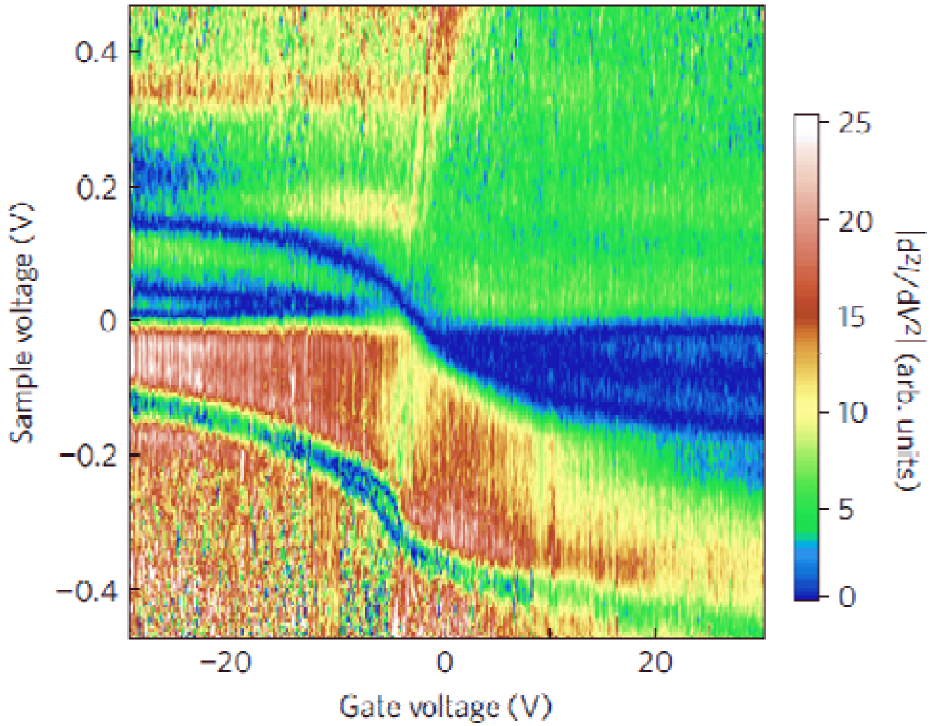






C. H. Park et.al. Nature Phys. 2008

Emergence of superlattice Dirac points in graphene on h-BN

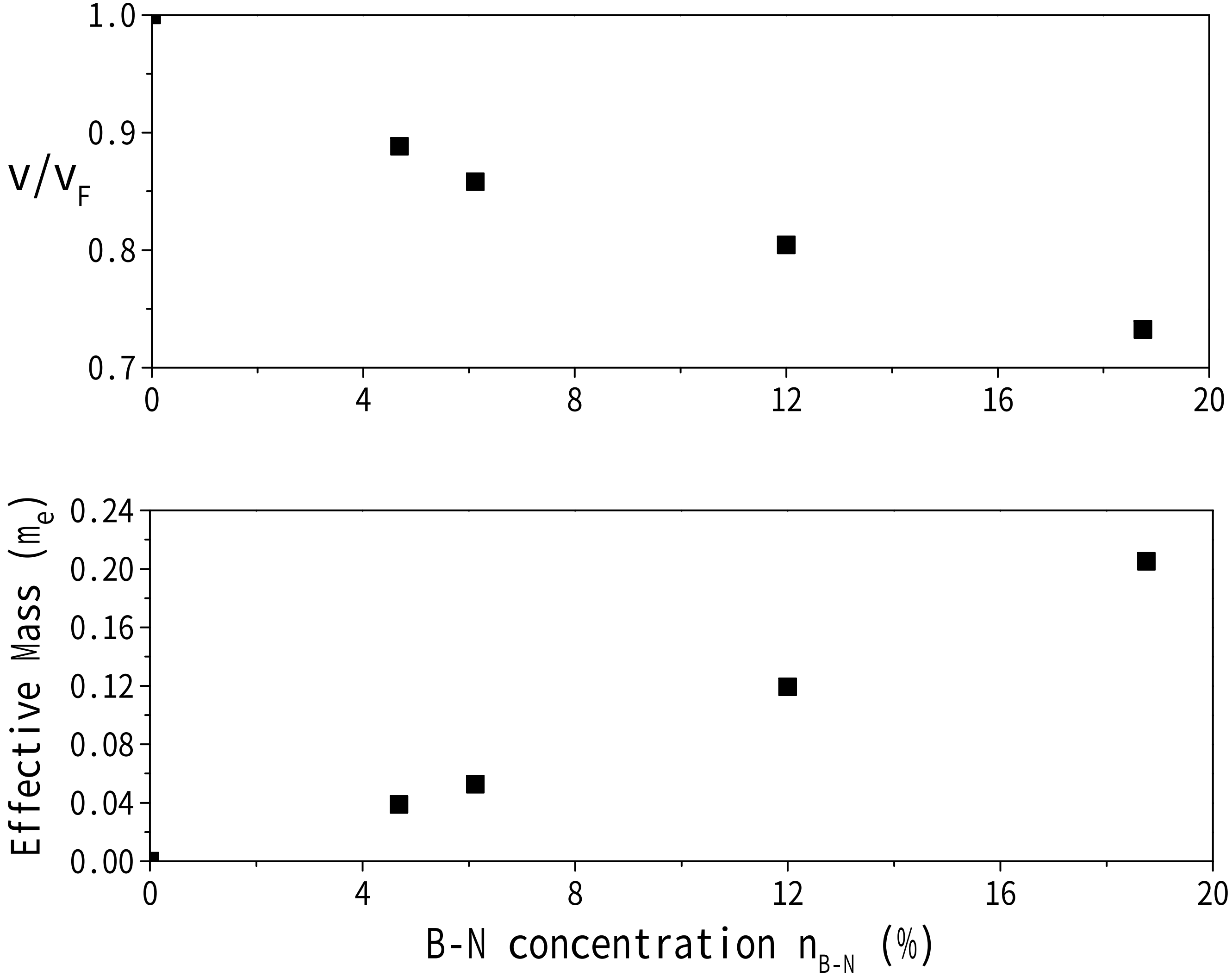


$$E_D = \hbar v_F \sqrt{2\alpha\pi(V_g - V_o)/g_v}$$

g_v : Valley degenecy

$V_g\ /V_0$: Gate/offset voltage

M. Yankowitz et.al. Nature Phys. 2012



1.0
0.9
0.8
0.7
v/v_F
0
4
8
12
16
20
0.24
0.20
0.16
0.12
0.08
0.04
0.00
Effective Mass (m_e)
0
4
8
12
16
20
B-N concentration n_B-N (%)

Summary

1. The phase separation between B-N domain and graphene is energetic by minimizing the number of C-B and C-N bonds at boundary .

2. The gap induced by symmetry broken is studied, a linear relation as B-N concentration at dilute limit is verified from experiment by XANES. At high doping level, the quantum confinement effect is dominant.

3. The anisotropy behavior of Dirac mass fermion is observed in h-BNC system, analogy to graphene under periodic potential , caused by periodic array of B-N dopants.

Acknowledgement

中研院原分所

Dr. Mei-Yin Chou 周美吟

Dr. Ching-Ming Wei 魏金明

台大物理所

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