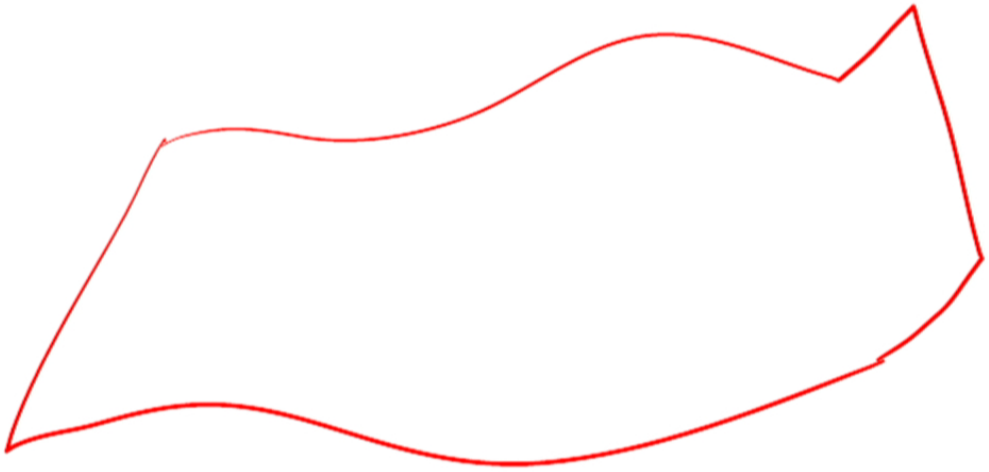
Title: Silicene - a Wonder Electron Carpet

Date: Oct 29, 2013 03:30 PM

URL: http://pirsa.org/13100128

Abstract: Graphene is a 2
dimensional net of strongly bonded carbon atoms. This magic carpet has taken us to new heights in the last decade. Silicene and Germanene are analogue nets, made of silicon and germanium atoms respectively, but with a relatively weaker chemical bond. I will argue that these carpets perform some new tricks by not being a carbon copy of graphene. We have suggested [1] that silicene and germanene are Mott insulators and potential abode for room temperature superconductivity, quantum spin liquids and more

Silicene - a Wonder Electron Carpet



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Acknowledgement

Akbar Jafari (Tehran), R Shankar, V Lukose
S Pathak (UC Santacruz), V Shenoy (IISc)
Krishnendu Sengupta (IACS)

for collaboration on various aspects of Graphene

Room temperature superconductivity, spin liquid and Mott Insultor: Silicene and Germanene as prospective playgrounds

G Baskaran, arXiv:1309.2242

Room temperature superconductivity, spin liquid and Mott Insultor: Silicene and Germanene as prospective playgrounds

G Baskaran, arXiv:1309.2242

Introduction

Graphene
Magic Electronic Carpet

Silicene & Germanene
Atomic radii, sp^3 mixing, puckered sigma bonds

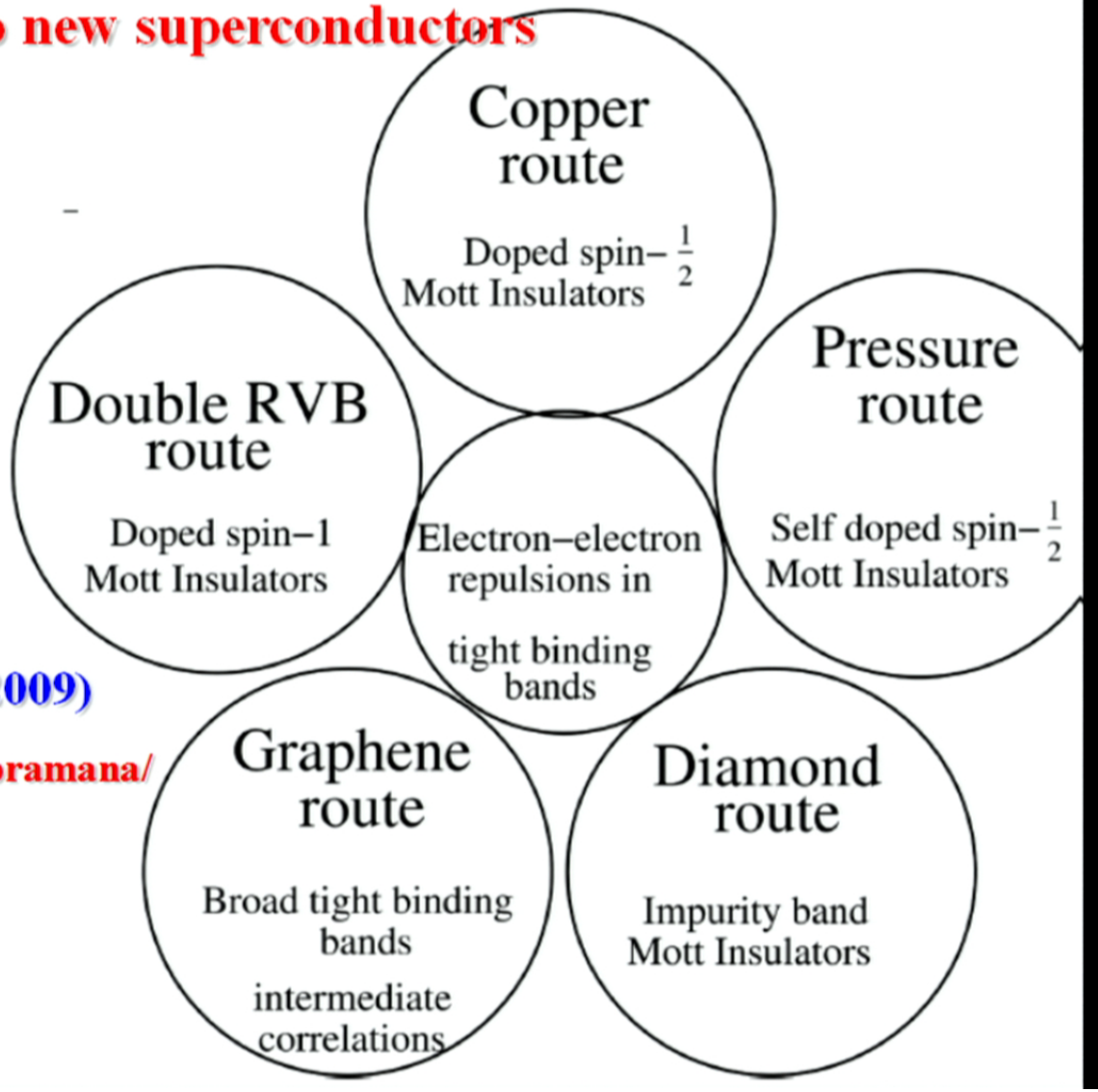
Bond Stretching
Stable Si_6H_6 ? Stable free standing Silicene ?

Why silicene should be a Mott insulator ?
Theory & Phenomenological support

Heisenberg Model, Dopped Mott insulator, tJ model ...
Synthesis of theory and experiment

Spin liquid, Prospects for Room Temperature Superconductivity

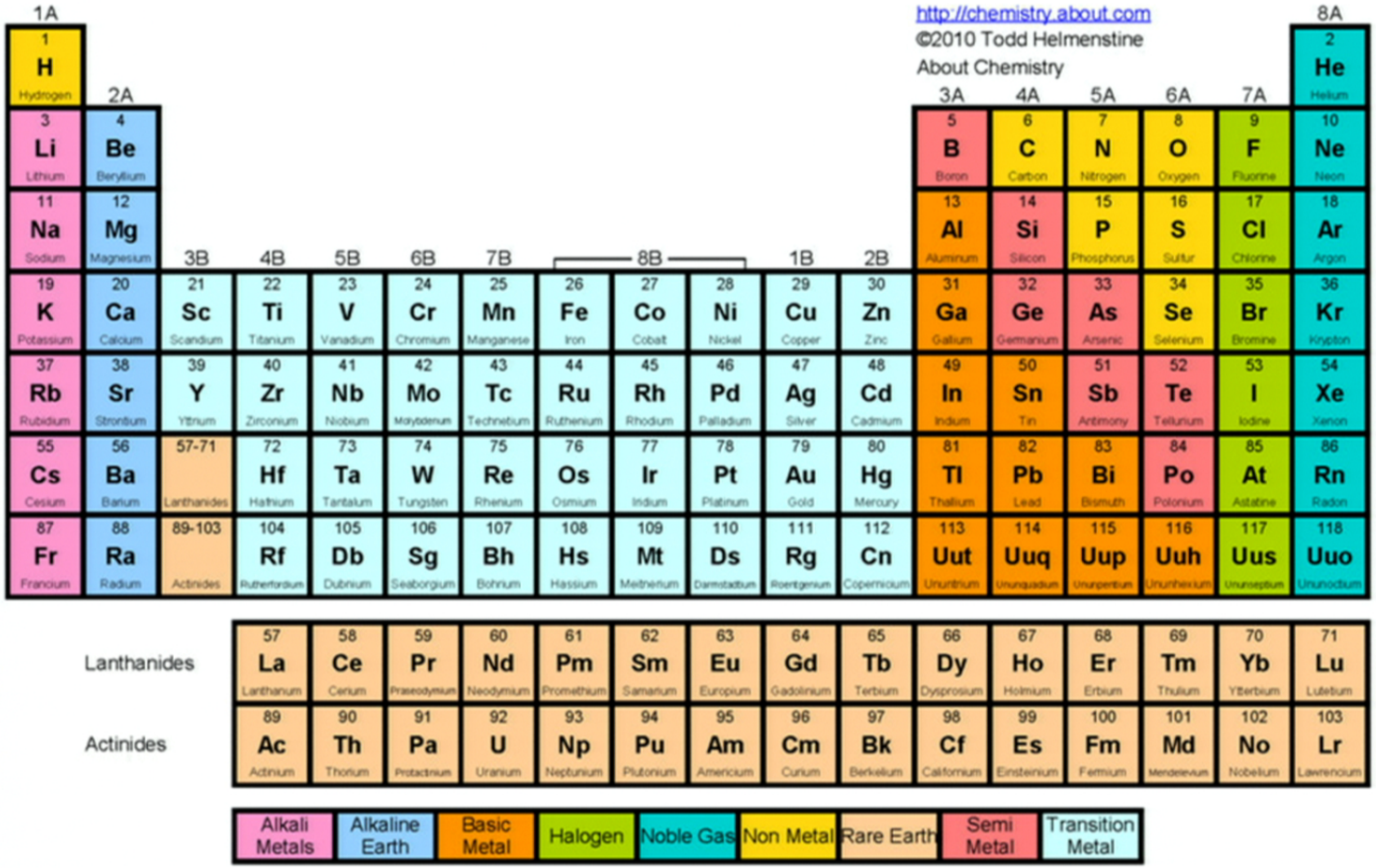
Five fold way to new superconductors



G Baskaran
Pramana 73, 61 (2009)

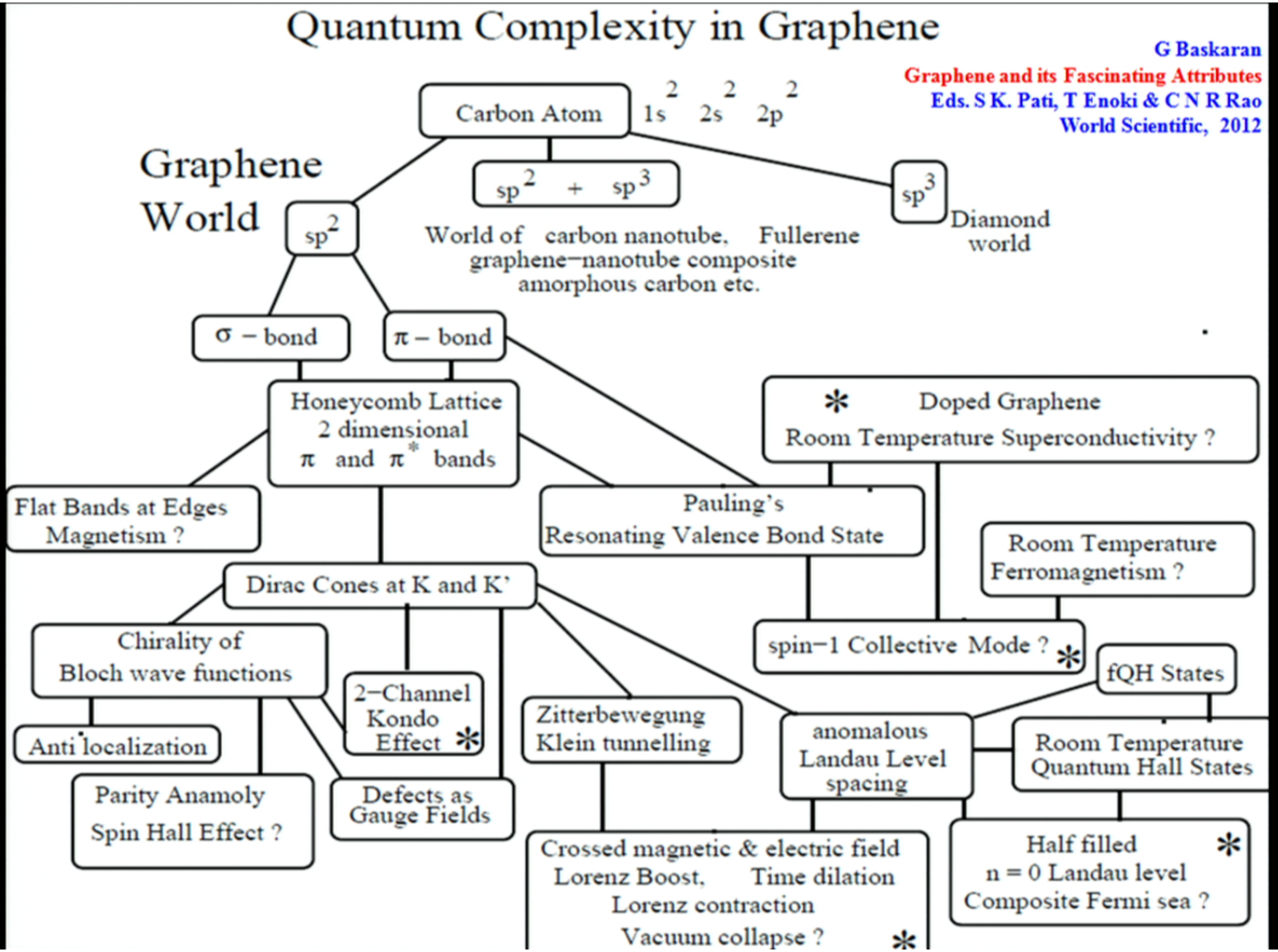
http://www.ias.ac.in/pramana/

Periodic Table of the Elements



Quantum Complexity in Graphene

G Baskaran
Graphene and its Fascinating Attributes
Eds. S K. Pati, T Enoki & C N R Rao
World Scientific, 2012



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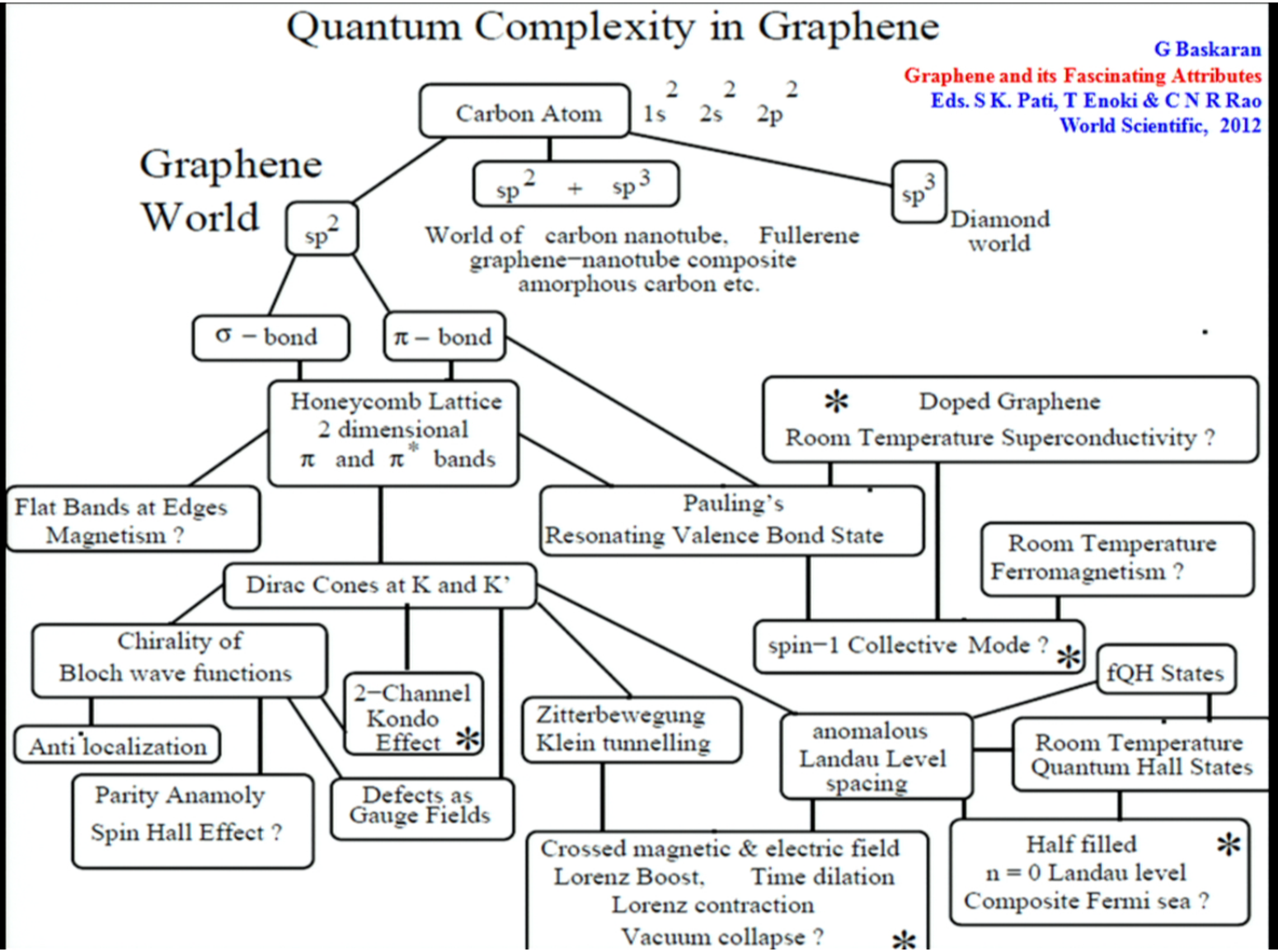
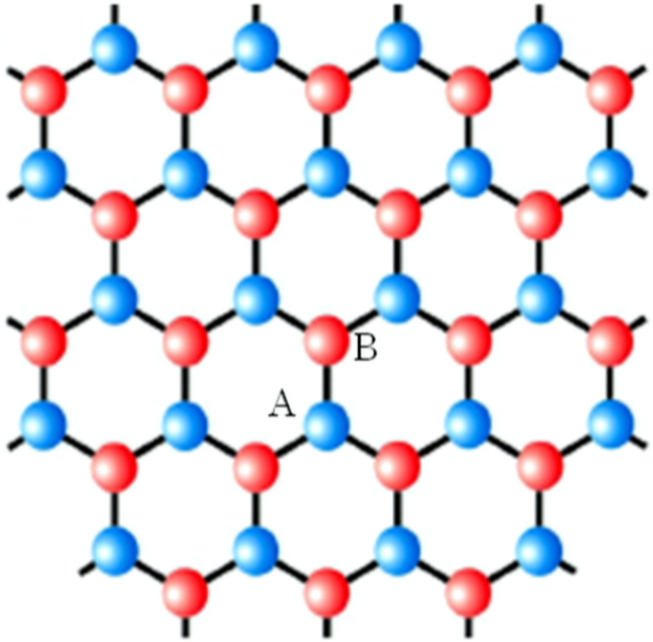


Basics

- **A single graphene layer : honeycomb lattice with two atoms (A & B) per unit cell**



– Carbon has 6 electrons
  - 2 are core electrons ($1s^2$)
  - 4 are valence electrons
    - one 2s orbital
    - three 2p orbitals

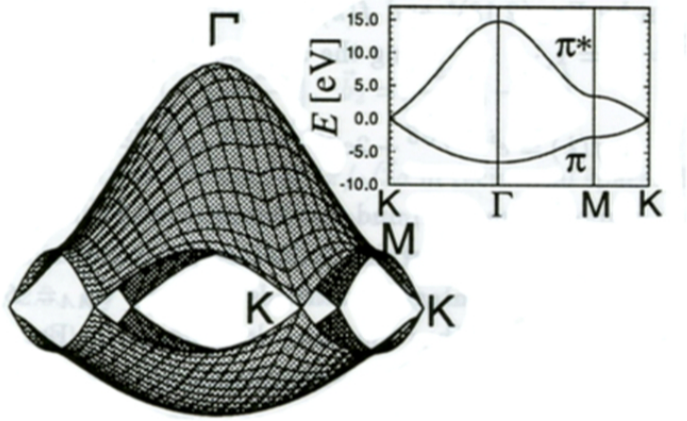
Band structure

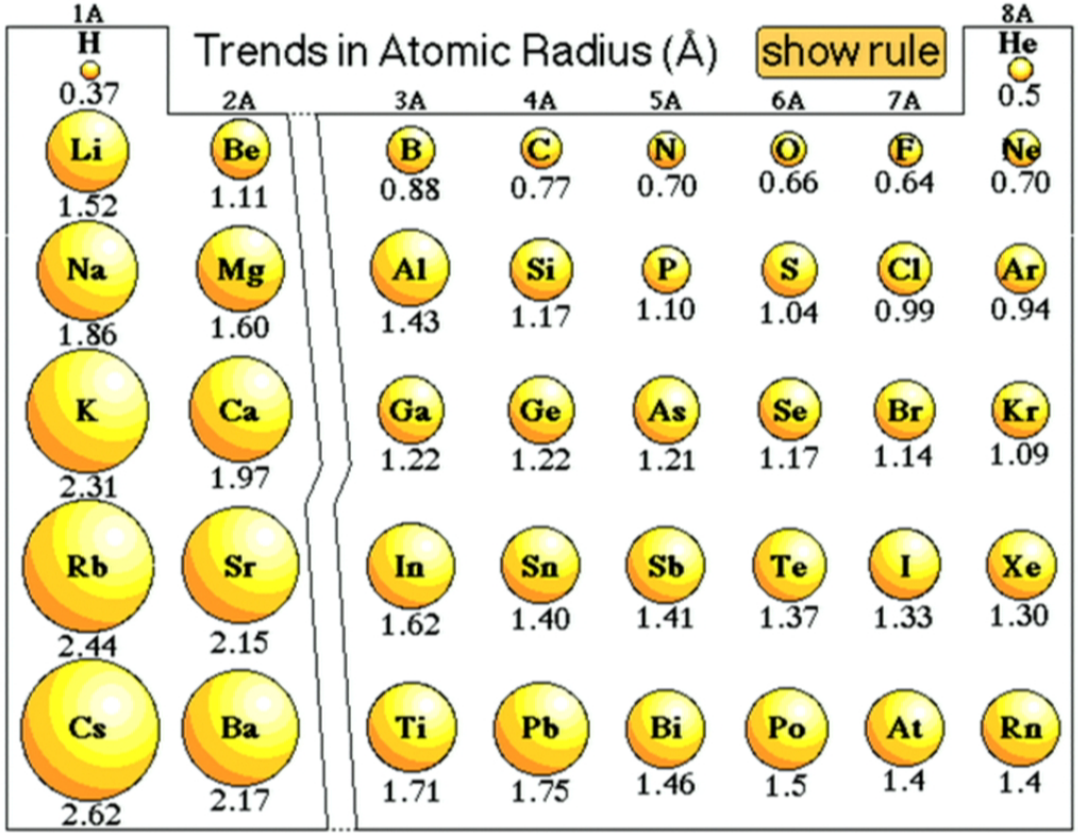
- Tight-binding model; nearest-neighbor interaction

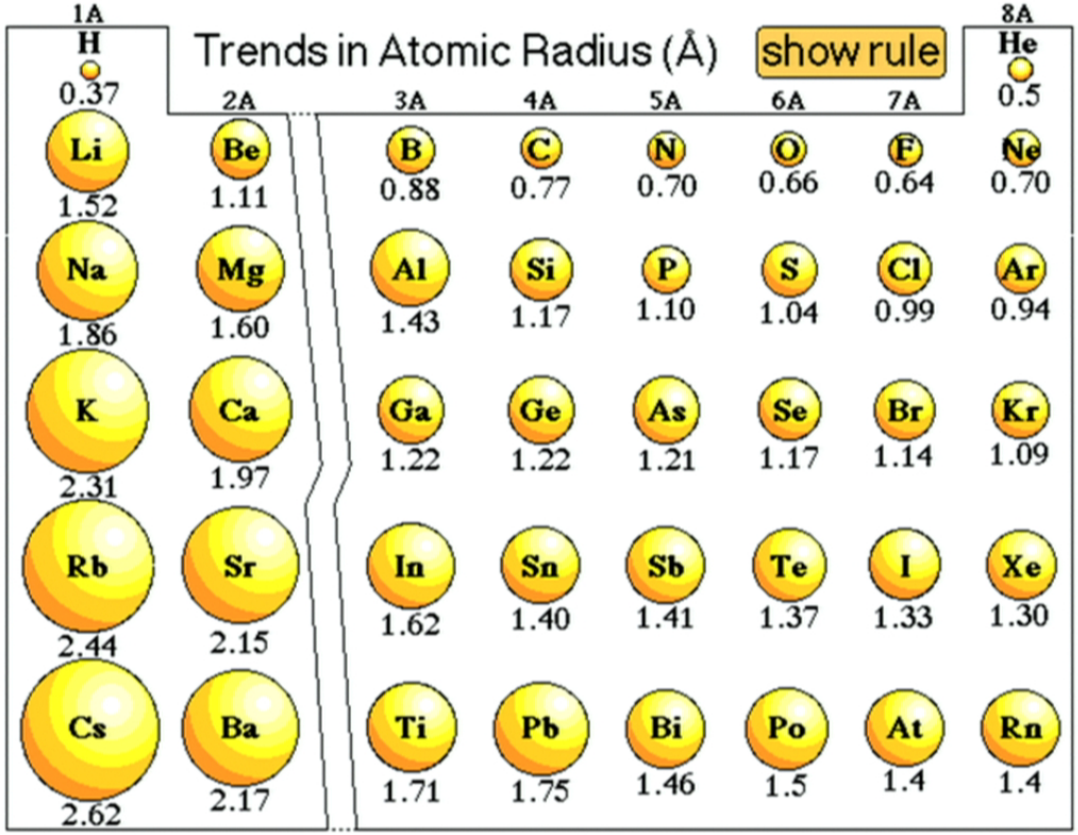
Wallace, PR 71,622 (1947)

$$E(k_x,k_y)=\pm t\sqrt{1+4\cos\left(\frac{\sqrt{3}k_y a}{2}\right)\cos\left(\frac{k_x a}{2}\right)+4\cos^2\left(\frac{k_x a}{2}\right)}$$

$t \approx 2.5$ eV overlap integral between nearest neighbors




Trends in Atomic Radius (Å)
show rule
1A
2A
3A
4A
5A
6A
7A
8A
H 0.37
He 0.5
Li 1.52
Be 1.11
B 0.88
C 0.77
N 0.70
O 0.66
F 0.64
Ne 0.70
Na 1.86
Mg 1.60
Al 1.43
Si 1.17
P 1.10
S 1.04
Cl 0.99
Ar 0.94
K 2.31
Ca 1.97
Ga 1.22
Ge 1.22
As 1.21
Se 1.17
Br 1.14
Kr 1.09
Rb 2.44
Sr 2.15
In 1.62
Sn 1.40
Sb 1.41
Te 1.37
I 1.33
Xe 1.30
Cs 2.62
Ba 2.17
Ti 1.71
Pb 1.75
Bi 1.46
Po 1.5
At 1.4
Rn 1.4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At 1.4
Rn 1.4

Silicene and Germanene

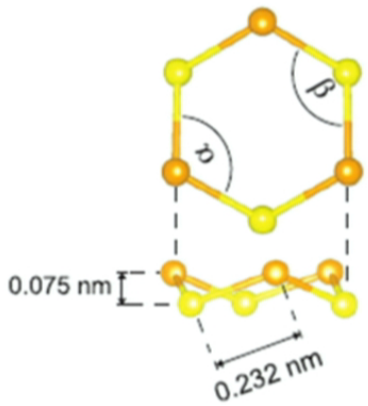
are Graphene analogue

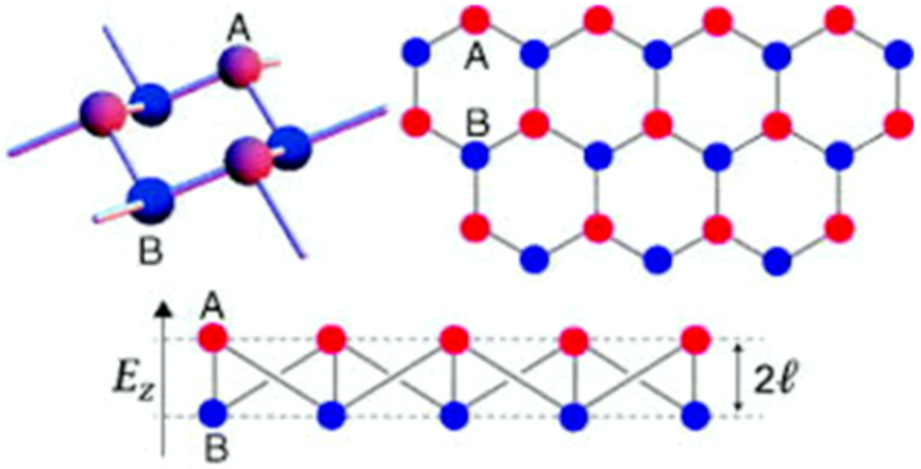
with Carbon being replaced by Si or Ge

Sp^2 bonding with a small **Sp^3 admixture**

Atom	Atomic radius	Bond Length
Carbon	0.77 Au	1.4 Au (graphene)
Silicon	1.17 Au	2.3 Au (silicene)
Germanium	1.22 Au	2.4 Au (germanene)

Graphene to Silicene, a 60 % bond stretch


β
α
0.075 nm
0.232 nm


A
B
A
B
A
B
E_z
2ℓ

Hexasilabenzene Si_6H_6 ?

a Silicon analogue of Benzene C_6H_6

Silicene is an infinite extension of hexalilabenzene

Is free standing silicene stable ?

Reduced aromaticity and radicalization

Sheka, Hoffmann

Radicalization in Molecules

O_2 , NO, polyanilene, …

Vs

Mott Localization in Solid

A periodic array of weakly coupled dangling bonds, spin-half moments

La_2CuO_4 , Si (111) surface

delocalized radicals as low energy spinons

of a Mott insulator

(GB 2013)

Radicalization in Molecules

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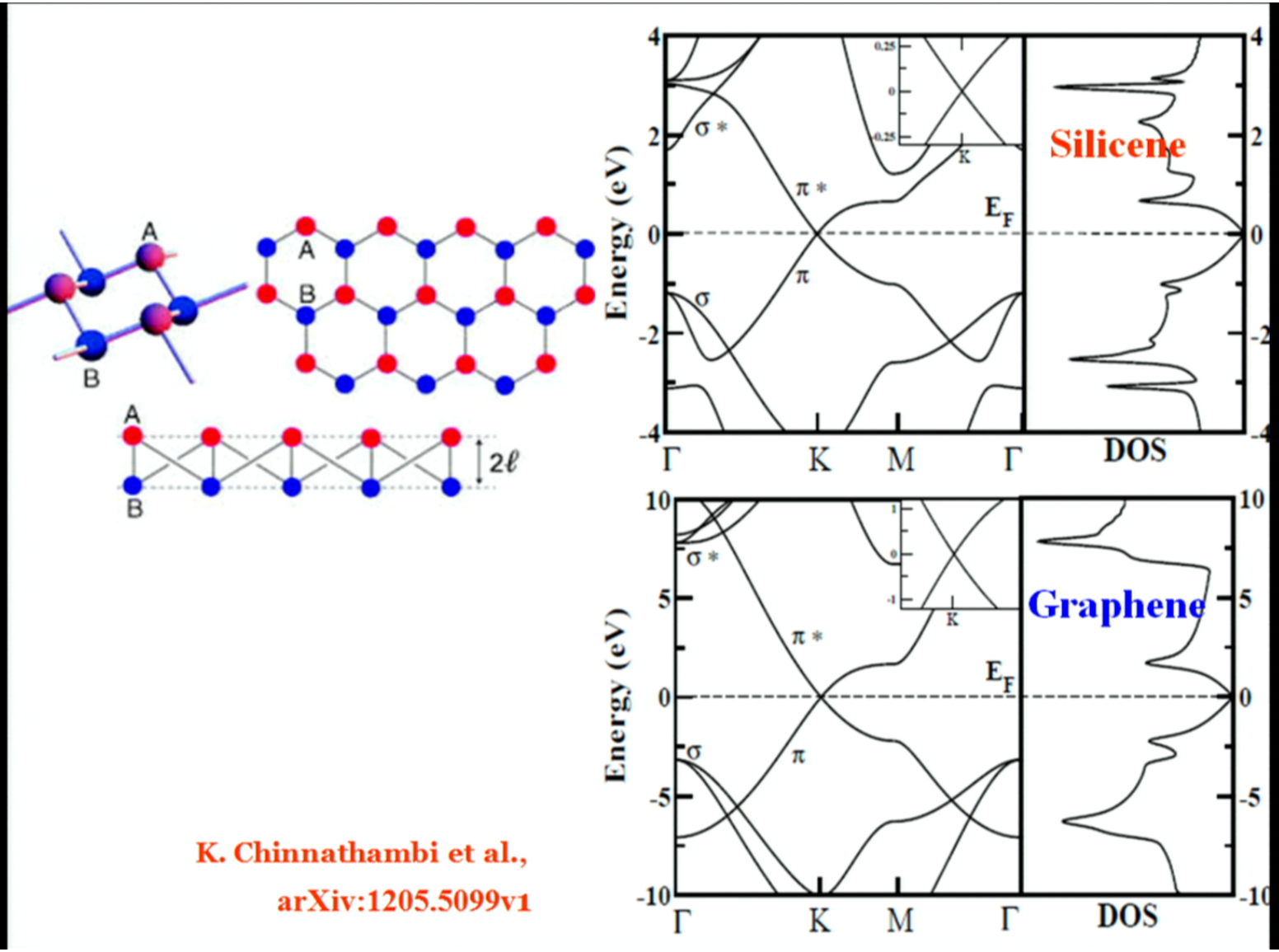
delocalized radicals as low energy spinons

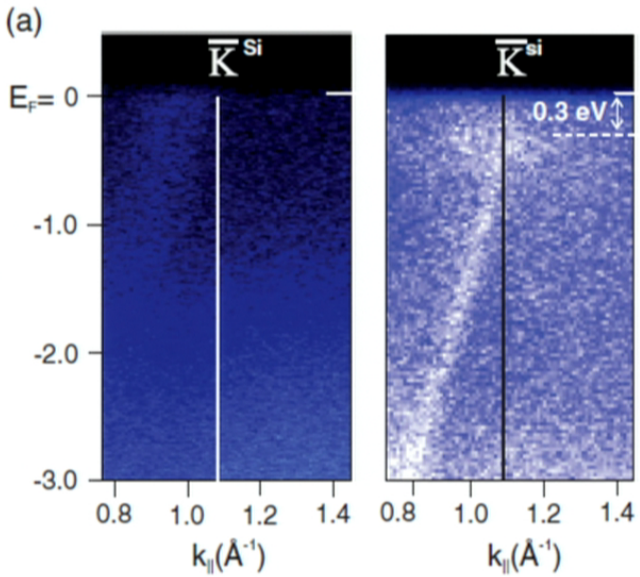
of a Mott insulator

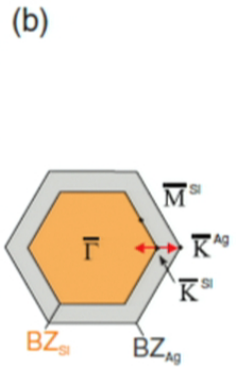
(GB 2013)

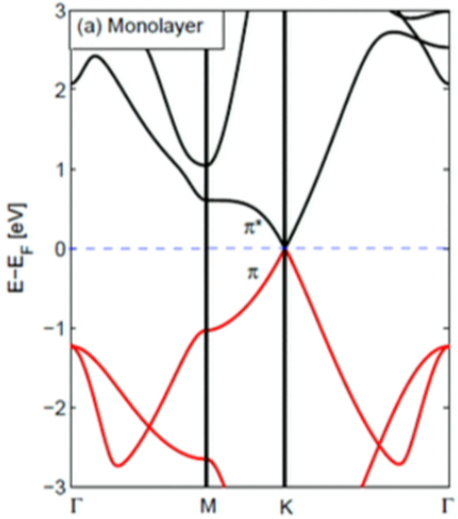
Free standing silicene has not been seen experimentally. As mentioned earlier stable silicene on metallic substrates, Ag, Ir and ZrB_2 have been synthesized. A possible key role of metallic substrate in stabilizing a silicene mono layer seen in experiments is an important issue that needs to be addressed further.


A
B
A
B
A
B
2ℓ
Energy (eV)
σ *
π *
σ
π
E_F
Γ
K
M
Γ
DOS
Silicene
Graphene
K. Chinnathambi et al.,
arXiv:1205.5099v1

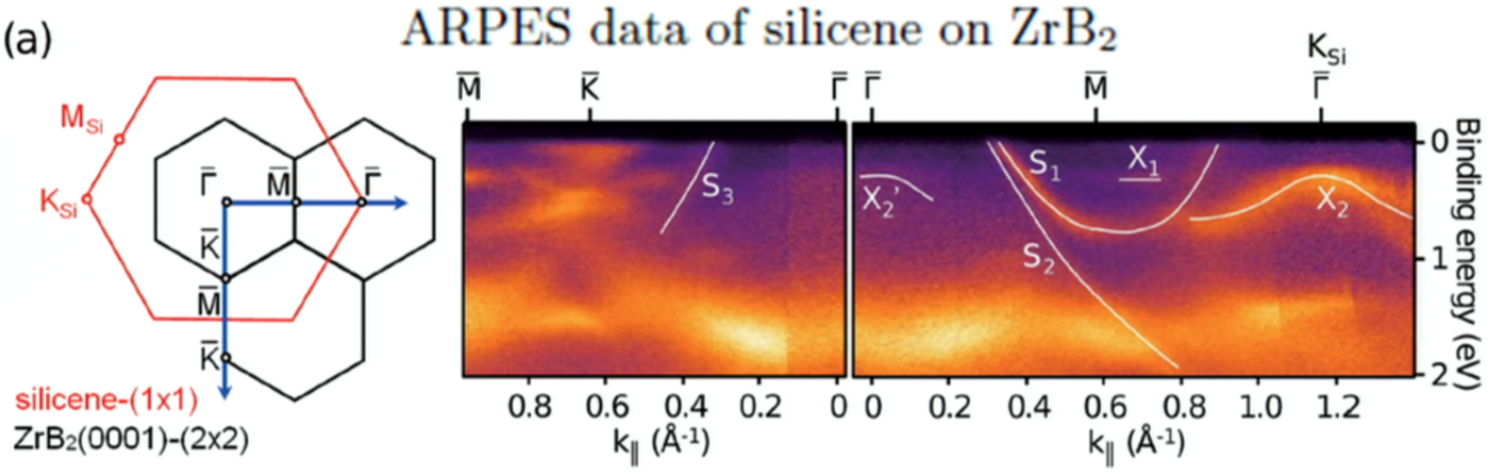
Silicene on Ag (111) surface Diract Cone ?



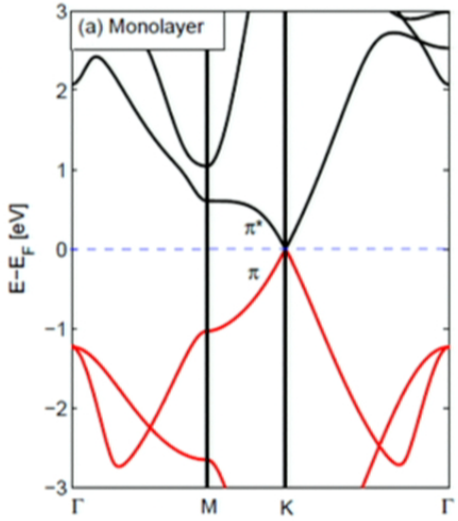




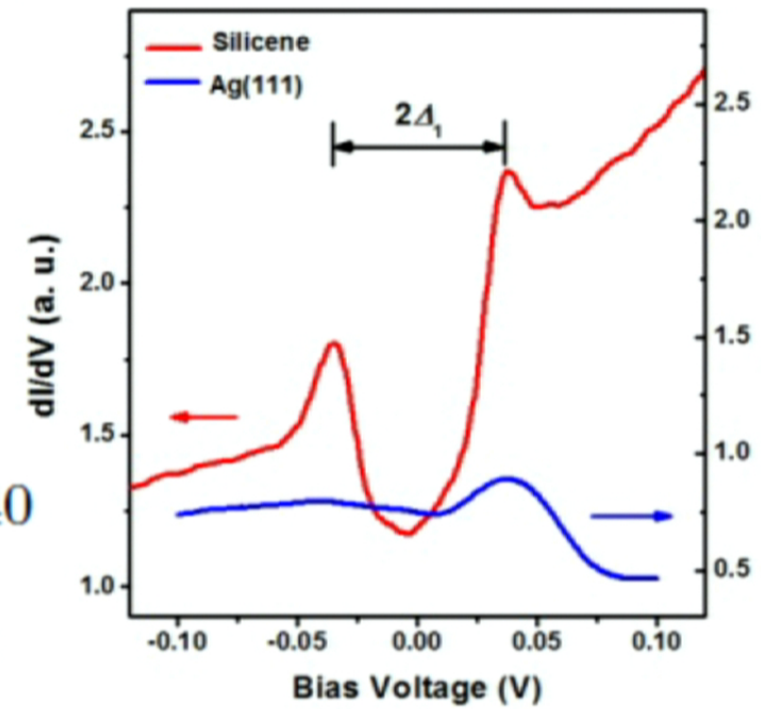
Vogt et al., PRL **108,** 155501 (2012)



A. Fleurence, R. Friedlein, T. Ozaki, H. Kawai, Y. Wang, Y. Yamada-Takamura, Experimental evidence for epitaxial silicene on diboride thin films. Phys Rev Lett **108**, 245501 (2012)



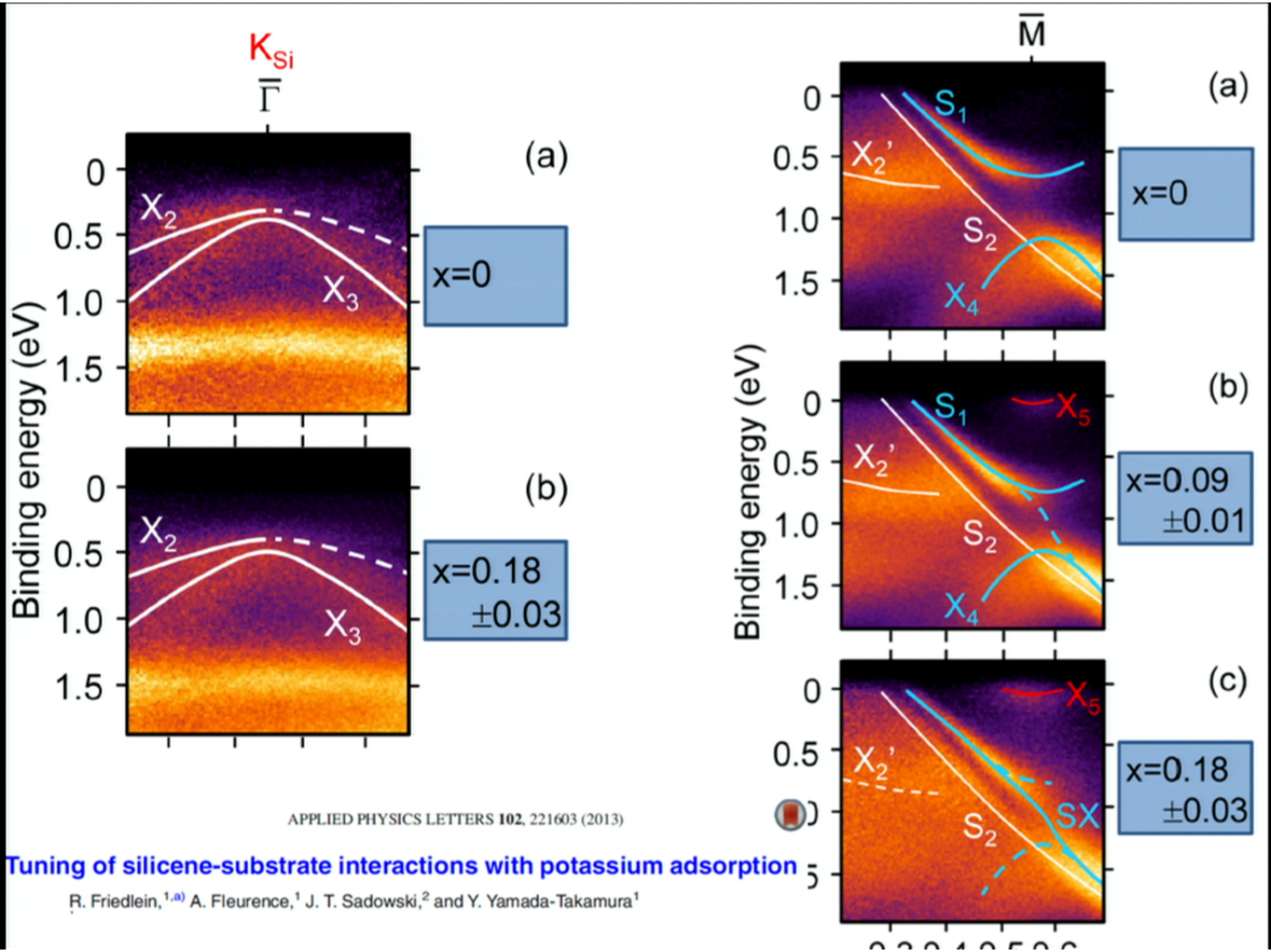
A Superconducting Gap Anomaly



Tc $\sim$ 35 to 40

$$\frac{2\Delta}{kT_c} \sim 20$$

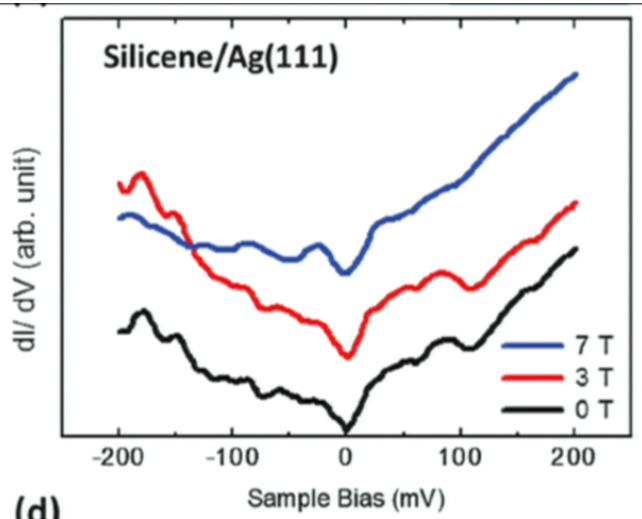
L. Chen, B. Feng, and K. Wu, Observation of a possible superconducting gap in silicene on Ag(111) surface, , App. Phys. Lett., **102**, 081602 (2013)



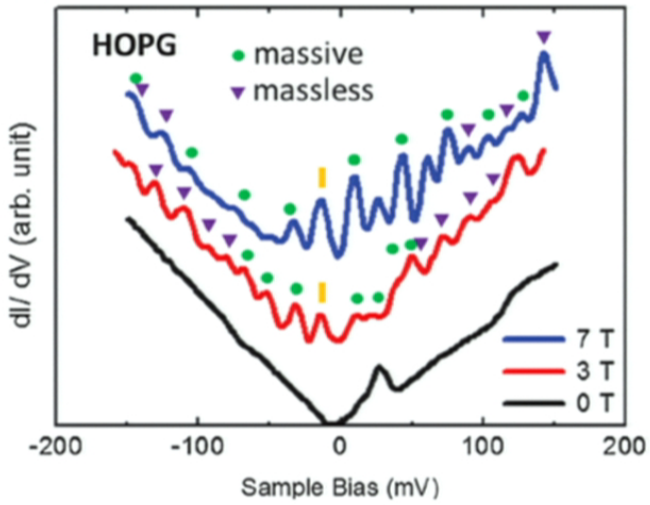
APPLIED PHYSICS LETTERS **102**, 221603 (2013)

Tuning of silicene-substrate interactions with potassium adsorption

R. Friedlein,[1,a)] A. Fleurence,[1] J. T. Sadowski,[2] and Y. Yamada-Takamura[1]

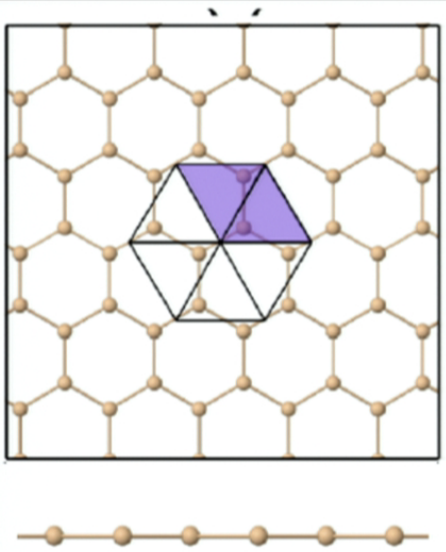


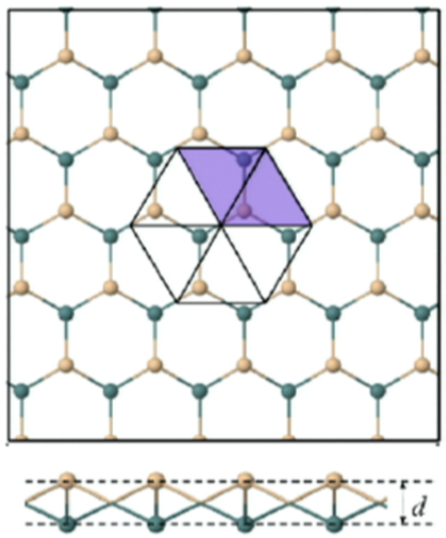
(d)

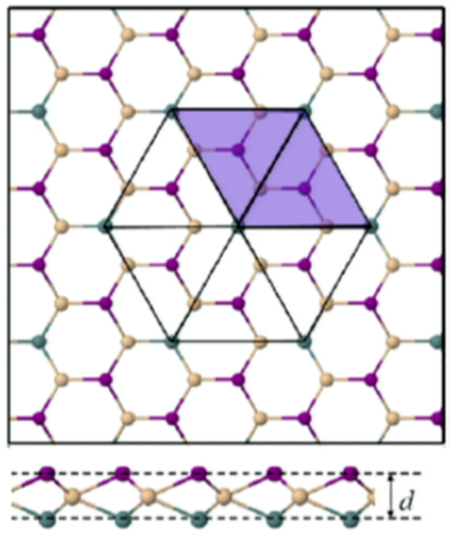


PRL **110,** 076801 (2013)

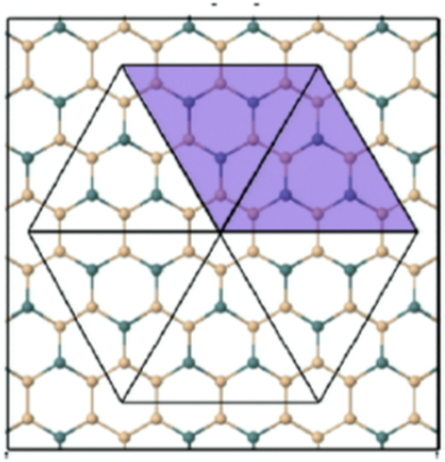
Chun-Liang Lin,[1] Ryuichi Arafune,[2] Kazuaki Kawahara,[1] Mao Kanno,[3] Noriyuki Tsukahara,
Emi Minamitani,[4] Yousoo Kim,[4] Maki Kawai,[1,3] and Noriaki Takagi[1,3,*]







$(\sqrt{3} \times \sqrt{3})$ unit cell



(4×4) unit cell.

Mott's argument

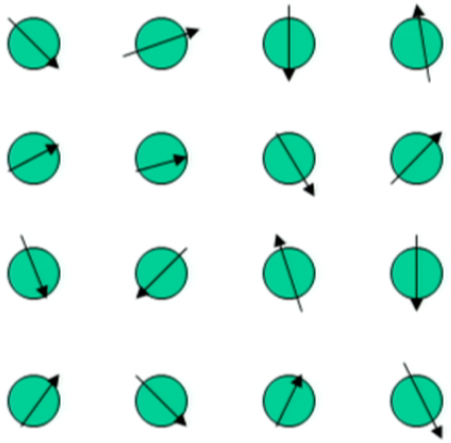
As we expand the lattice of a half filled band of electrons coulomb screening will get reduced

When will an electron form a quantum mechanical bound state with the hole it left behind at its home site ?

When a bound state is formed some free electrons will disappear. This will reduce screening further and increase the binding energy – more free electrons will disappear

Thus there is a feed back leading to a first order phase transition

Let us expand the lattice



$a >> a_B$

For $a >> a_B$

we get a Mott insulator

upper Hubbard band

Spins are soft degrees of freedom while charges are frozen

lower Hubbard band

Mott's argument

As we expand the lattice of a half filled band of electrons coulomb screening will get reduced

When will an electron form a quantum mechanical bound state with the hole it left behind at its home site ?

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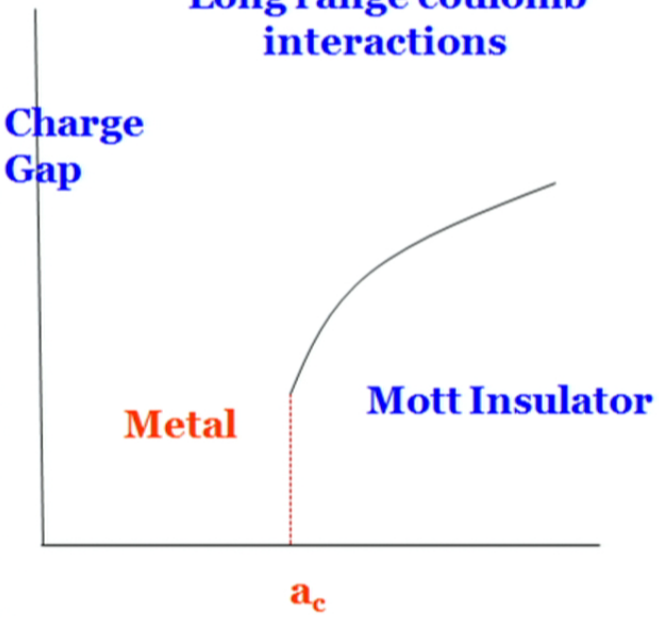
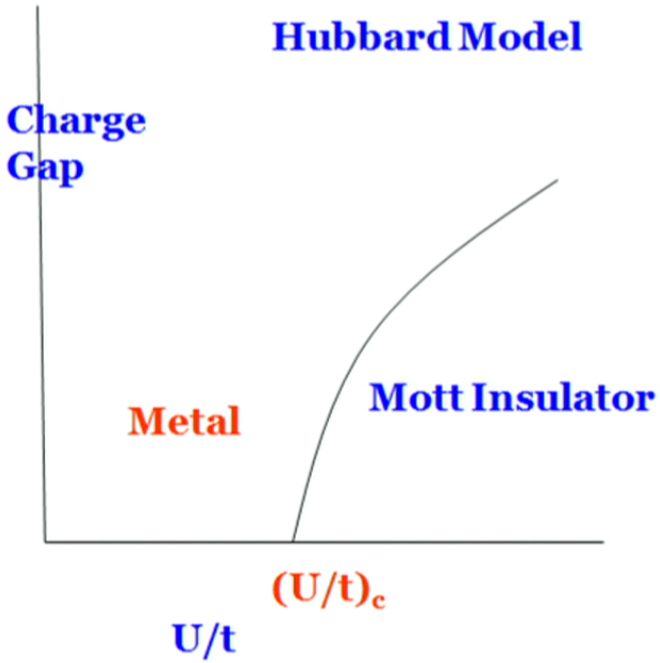
Thus there is a feed back leading to a first order phase transition

$$H = -t \sum_{\langle ij \rangle} C^{\dagger}_{i\sigma} C_{j\sigma} + \text{H.c.} + U \sum n_{i\uparrow} n_{i\downarrow}$$

Real systems with Long range coulomb interactions



Hubbard Model



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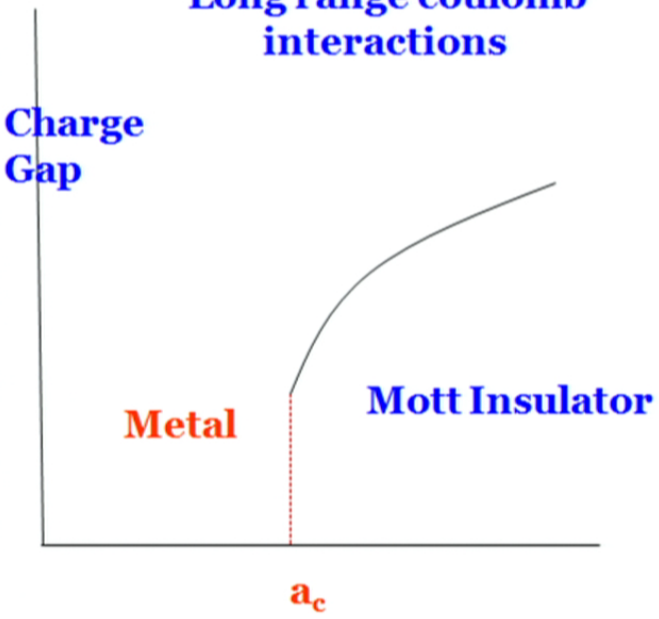
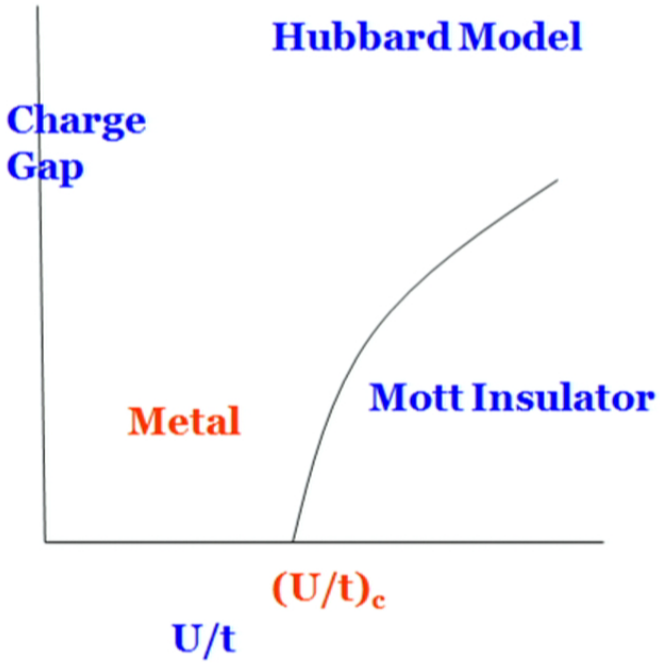
Real systems with Long range coulomb interactions



Hubbard Model



Mott (semi-metal to insulator) transition in a Hubbard Model On a Honeycomb Lattice

Sorella, Tosatti 1992

$$H = -t \sum_{\langle ij \rangle} C^{\dagger}_{i\sigma} C_{j\sigma} + \text{H.c.} + U \sum n_{i\uparrow} n_{i\downarrow}$$

Critical U/t ~ 3.8

a recent and more accurate estimate U/t ~ 4.1

Theoretical Support for Mott Insulating State in Silicene

GB 2013

Estimate for silicene $U/t \sim 4.1$

$V/t \sim 2.1$ Schuler et al. PRL 2013

This places silicene on the Mott insulating side
The onsite Hubbard U gets effectively enhanced

$$U^* \approx U + \alpha V$$

where $\alpha \sim 1$.

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where $\alpha \sim 1$.

Quantum Spin Liquids

$$H_s = J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4}) + 4 \text{ \& } 6 \text{ spin terms}$$

$\mathrm{t} \sim 1.14 \text{ eV}$

$\mathrm{U} \sim 5 \text{ eV}$

$\mathrm{J} \approx \frac{4t^2}{U^2} \approx 1 \text{ eV}$

Quantum Spin Liquids

$$H_s = J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4}) + 4 \text{ \& } 6 \text{ spin terms}$$

$\mathrm{t} \sim 1.14$ eV

$\mathrm{U} \sim 5$ eV

$\mathrm{J} \approx \frac{4t^2}{U^2} \approx 1$ eV

Dopped Mott Insulator tJ Model

$$H_{\mathrm{tJ}} = -t \sum_{\langle ij \rangle} (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.) + J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j)$$

$$n_{i\uparrow} + n_{i\uparrow} \neq 2 \text{ or } 0.$$

Superconductivity in Hubbard Model and tJ model on a Honeycomb lattice

T. C. Choy and B. A. McKinnon, Significance of nonorthogonality in tight-binding models. II. The possibility of high-Tc superconductivity in intercalation compounds, Phys. Rev. **B 52**, 14539 - 14543 (1995)

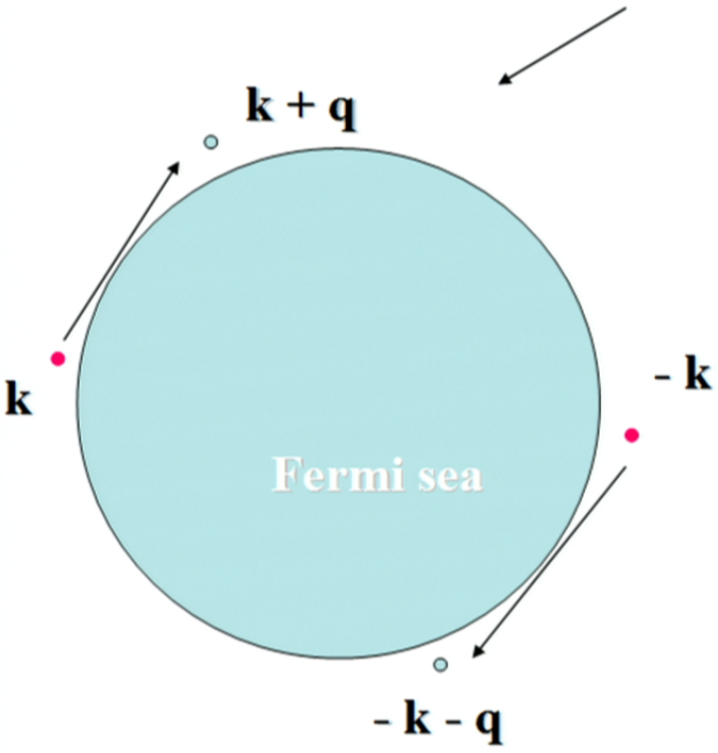
G. Baskaran, Resonating-valence-bond contribution to superconductivity in MgB2, Phys. Rev. **B 65**, 212505 (2002)

A. M. Black-Schaffer and S. Doniach, Resonating valence bonds and mean-field d-wave superconductivity in graphite, Phys. Rev. **B 75**, 134512 (2007)

S. Pathak, V. B. Shenoy, and G. Baskaran, Possible high-temperature superconducting state with a d+id pairing symmetry in doped graphene, Phys. Rev., **B 81**, 085431 (2010)

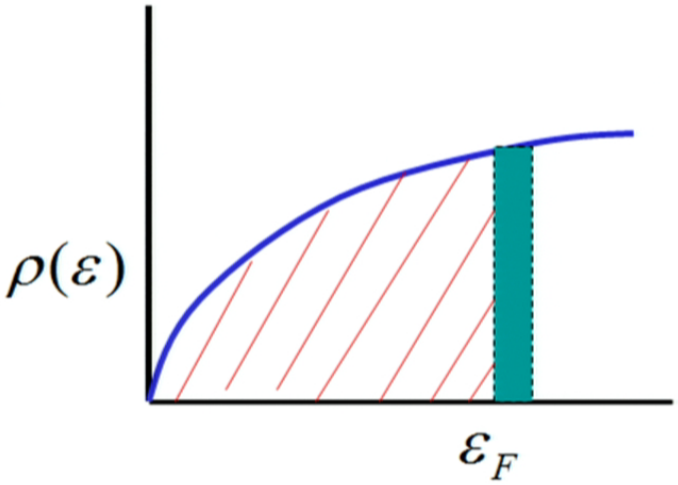
BCS theory of Superconductivity is based on a Fermi liquid reference state

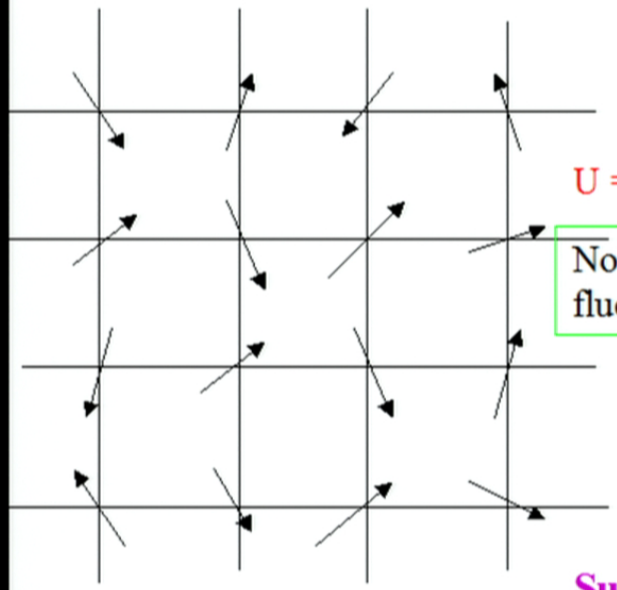
m*, fermi liquid parameters, ..



Fraction of participating electrons $\frac{\hbar\omega_D}{\varepsilon_F} << 1$

Severe Pauli Blocking

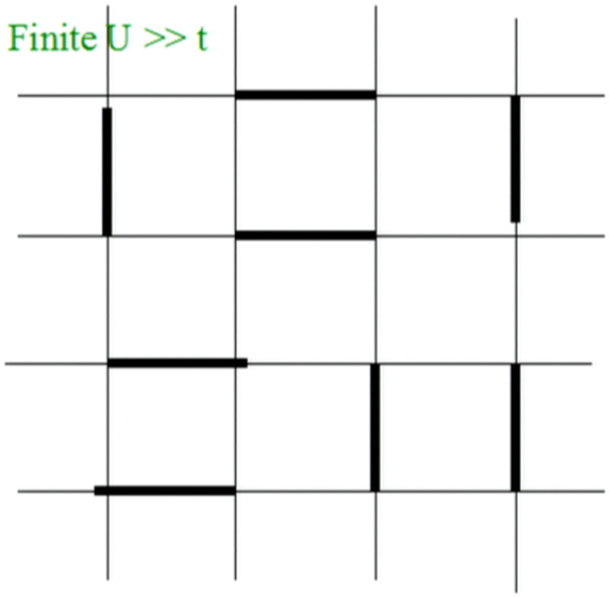




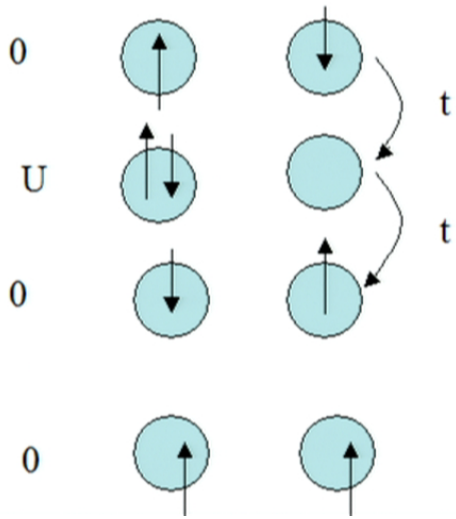
U = infinity

No quantum fluctuations

Finite U >> t



Superexchange or Kinetic exchange process

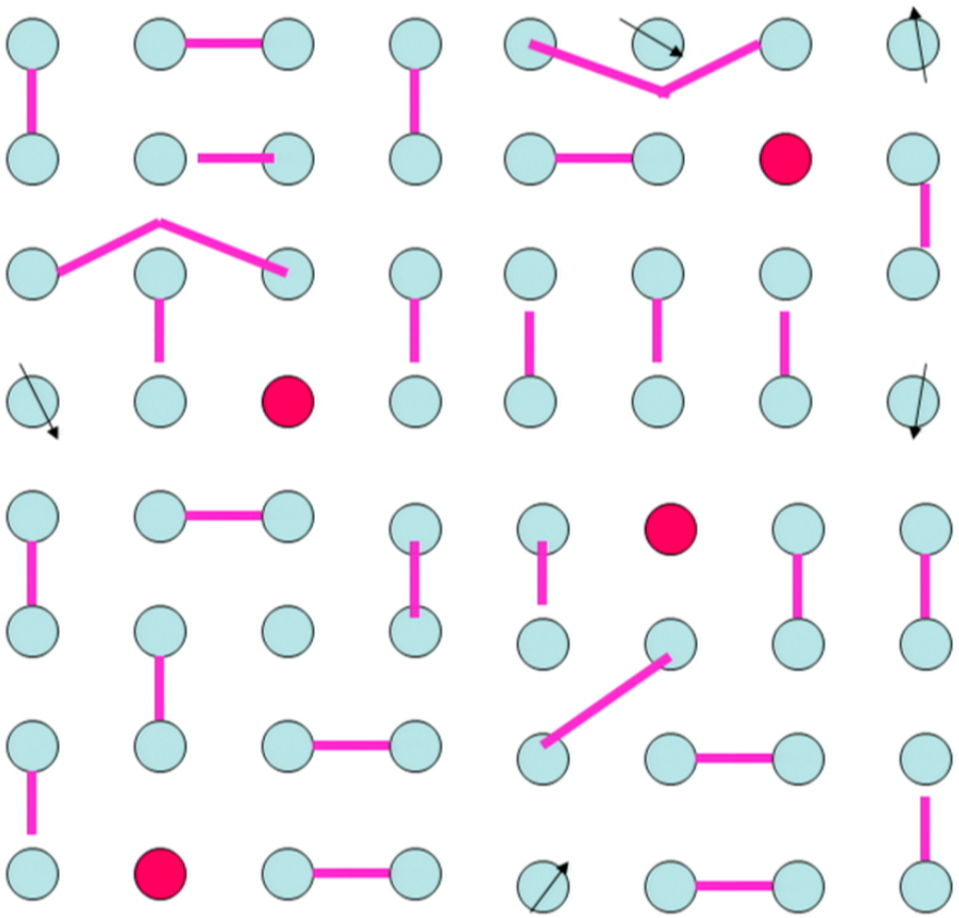


$$\text{Energy gain} = J = \frac{-4t^2}{U}$$

$$\text{Energy gain} = 0$$

$$\text{———} = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

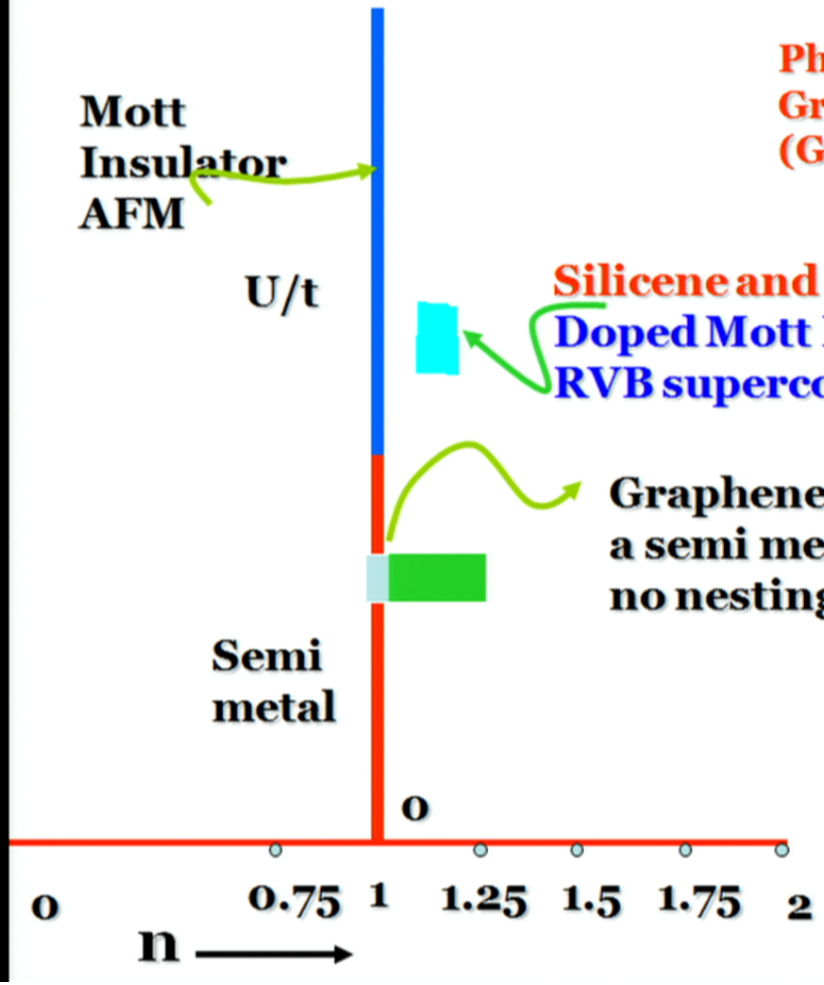
$$H = J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j - \tfrac{1}{4}\right)$$



Hubbard model

2D Honeycomb lattice

Phase Diagram for Graphene, Silicene and Germanene (GB 2013)



$$|\Psi\rangle = g^{\mathcal{D}}|BCS\rangle_N$$

$$\mathcal{D} = \sum_i (n_i^a + n_i^b)$$

Variational Monte Carlo **13 x 13 sites**

S Pathak, V Shenoy and GB, Phys. Rev. B (2010)

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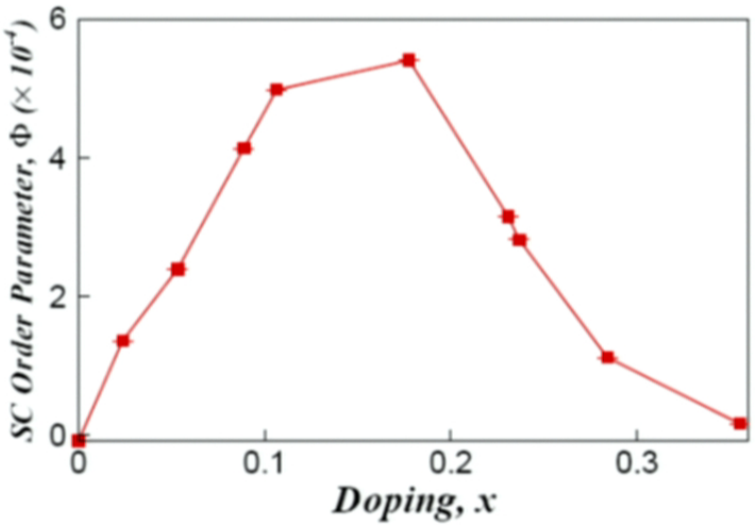

FIG. 1: Doping dependence of superconducting order parameter Φ as obtained from VMC calculation of the Hubbard model on a honeycomb lattice for $U/t = 2.4$.

$$k_b T_c = \frac{1}{1.764} \frac{\hbar v_F}{\pi \xi}$$

Kosterlitz-Thouless State

$$k_b T_c = \frac{t}{50}$$ **~200 to 400 K ?**

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Possibility of Room Temperature Superconductivity

GB 2013

(t, J) for cuprates $\longrightarrow$ 4 (t,J) for Silicene

we have an unusually large J $\sim$ 1 eV and t $\sim$ 1 eV for our honeycomb lattice. This is to be contrasted with a value of J $\sim$ 0.15 eV and t $\sim$ 0.25 eV for the square lattice cuprates, known for their record Tc $\sim$ 90° K, for for single layer cuprates. We have an average 4 fold fold increase in t and J for silicene. Does silicene offer a 4 fold increase in Tc ? Taking care of lattice structure difference between cuprate and silicene crudely, a scaling gives at least 3 fold increase of Tc. Thus room temperature scales for Tc seems within reach, provided competing orders are taken care of .

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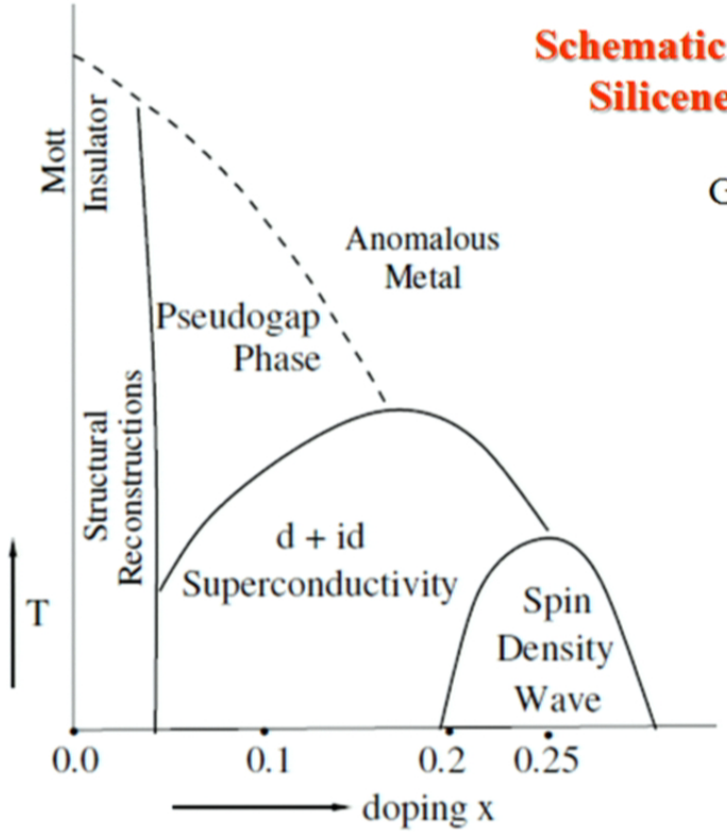
$$
\begin{aligned}
H &= K a_0^2 \sum_{\langle ij \rangle} \tau_i \tau_j - K_0 a_0^2 \sum_i \tau_i^2 - \\
&- \sum_{\langle ij \rangle} t(1 + \kappa_t a_0^2 (\tau_i - \tau_j)^2)(c_{i\sigma}^\dagger c_{j\sigma} + H.c.) + \\
&+ J \sum_{\langle ij \rangle} (1 + \kappa_J a_0^2 (\tau_i - \tau_j)^2)(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j)
\end{aligned}
$$

Schematic Phase Diagram for Silicene and Germanene

G Baskaran, arXiv:1309.2242



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