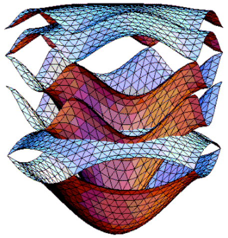
Yukawa International Seminar 2007 (YKIS2007)

Interaction and Nanostructural Effects in Low-Dimensional Systems

Nov.5-30, 2007, Yukawa Institute for Theoretical Physics



Excitonic Properties of single wall carbon nanotubes

R. Saito, K. Sato, J. S. Park,
齋藤　理一郎、佐藤　健太郎、박진성

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***UFMG, ***MIT, +Tokyo Univ. ++ Nagoya Univ.*

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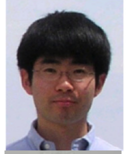
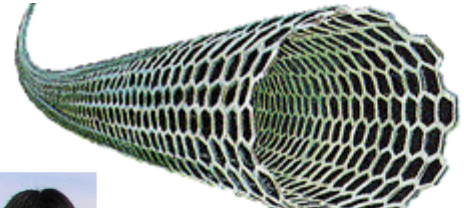
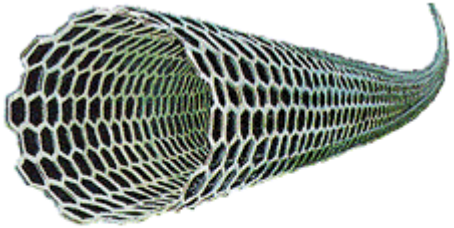
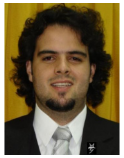








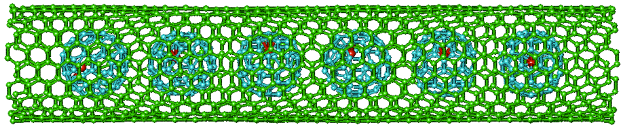


TOHOKU UNIVERSITY 東北大学 TOHOKU UNIVERSITY

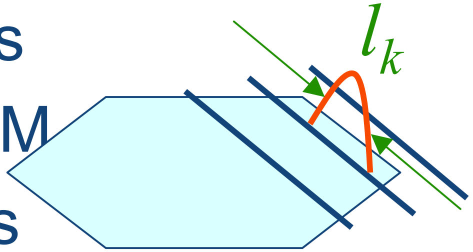
JST 科学技術振興機構 Japan Science and Technology Agency

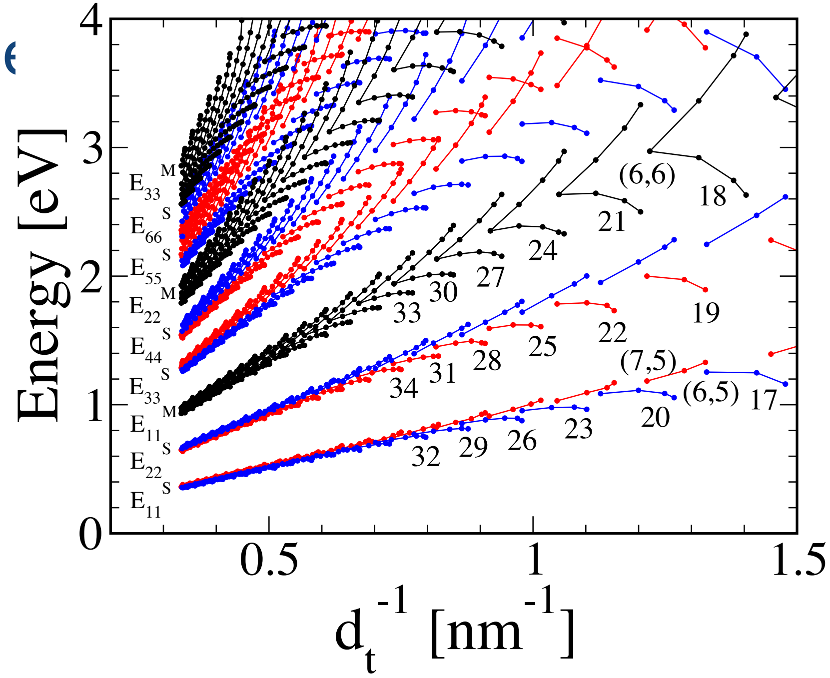
YKIS'07

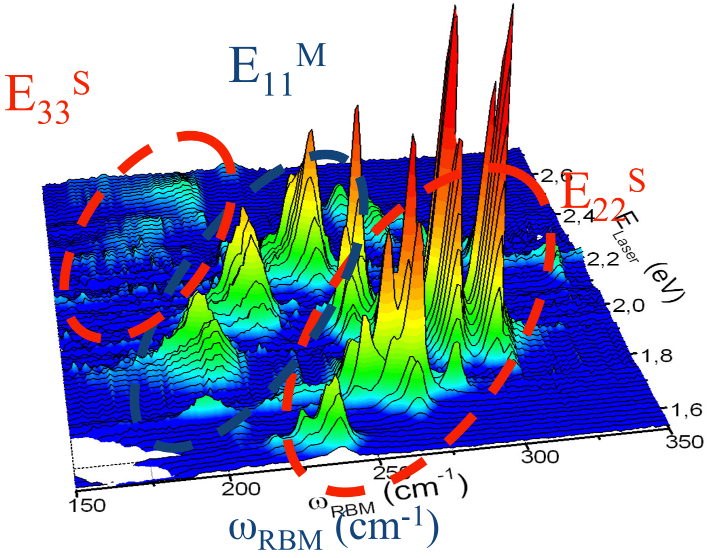
Outline of talk



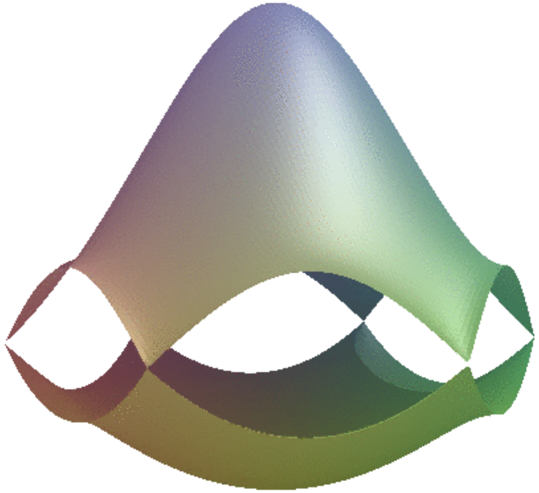
- Electron and Phonons of NTs
- ETB-Exciton calculation and related problems
  - for 0.6-3nm diameter up to E66S and E22M
  - E33S E44S, ..., E66s higher exciton states
  - e citons

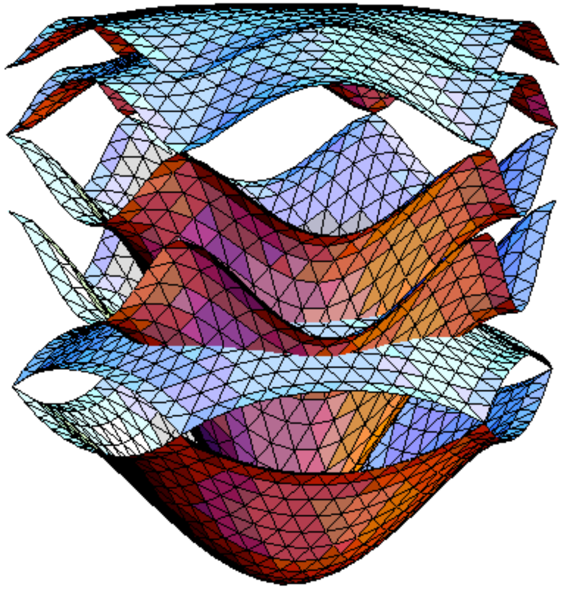


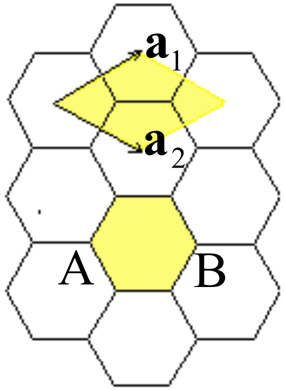




Electron and Phonons of Nanotubes

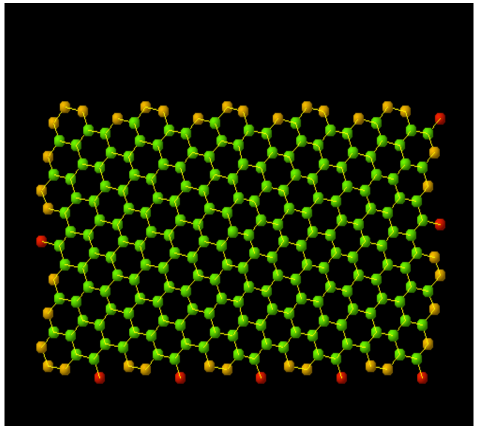






Chiral Vectors : *(n,m)*

R. Saito *et al., Phys. Rev*. B
46, 1804 (1992)



- Chiral Vector (equator of nanotube): OA, C_h
- Translational Vector of 1D material: OB, *T*
- Unit Cell : OAB'B

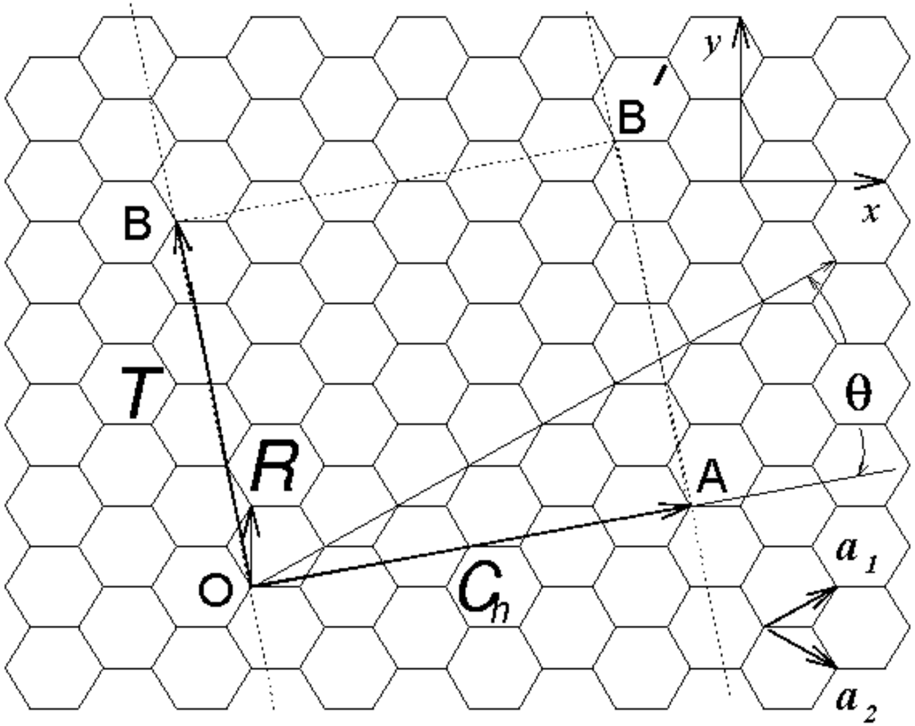
$$C_h = na_1 + ma_2 \equiv (n,m)$$

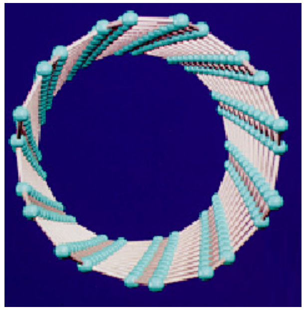
a_1, a_2 : primitive lattice vectors

$$T = t_1 a_1 + t_2 a_2 \equiv (t_1, t_2)$$

$$t_1 = \frac{(2m+n)}{d_R}, t_2 = -\frac{(2n+m)}{d_R}$$

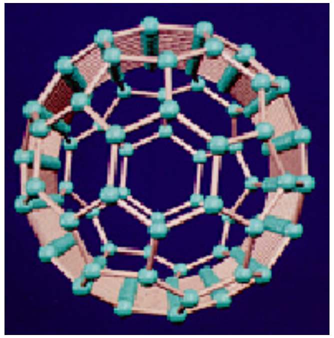
$$d_R = \gcd(2n+m, 2m+n)$$





Symmetry of Nanotube

M. S. Dresselhaus *et al.*,
Phys. Rev. **B45** 6234 (1992)



- Symmorphic (mirror symmetry)
  - Armchair Nanotube *(n,n)*, *n=m*
  - Zigzag Nanotube *(n,0)*, *m=0*
- Non-Symmorphic (axial chirality)
  - Chiral Nanotube *(n,m)*, $n \neq m$

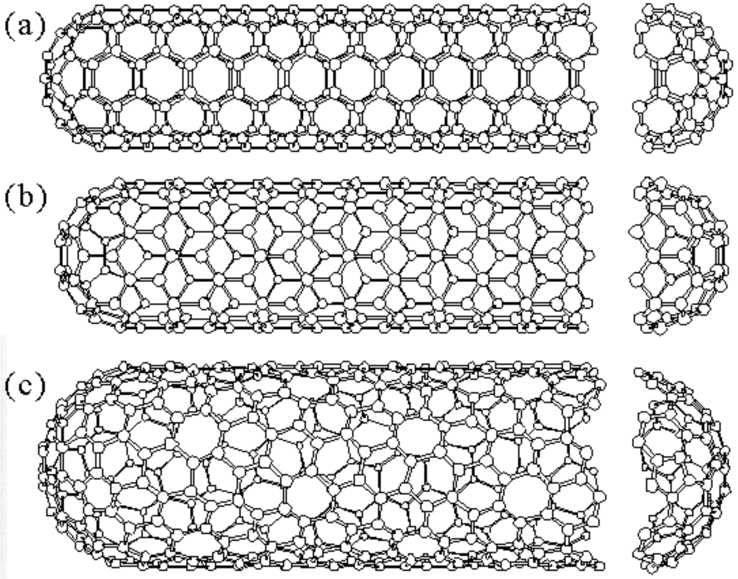
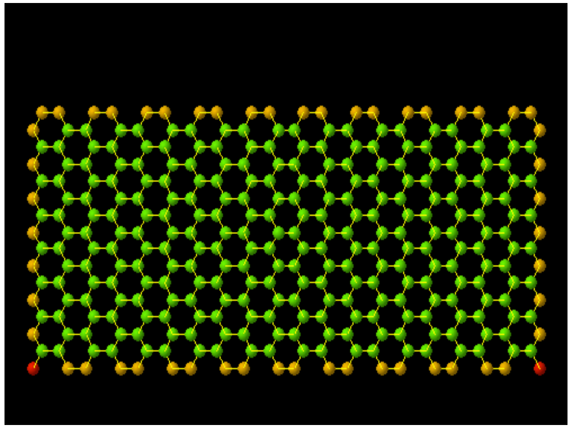
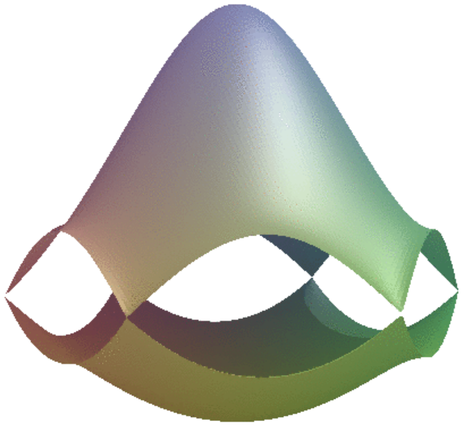


Fig: (a) (5,5) armchair,
(b) (9,0) zigzag, and
(c) (10,5) chiral nanotubes

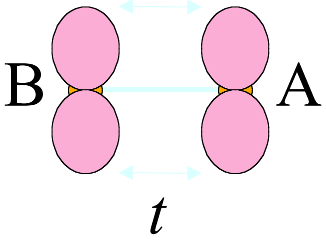


(10,10)
armchair
nanotube

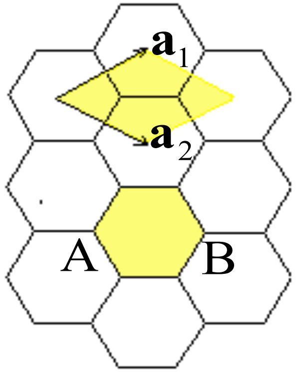


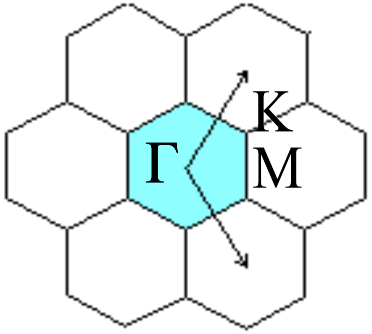
Energy band of Graphite

P. R. Wallace, *Phys. Rev*, **71** 622 (1947).



- π band of graphite
  - Unit Cell, B. Z.

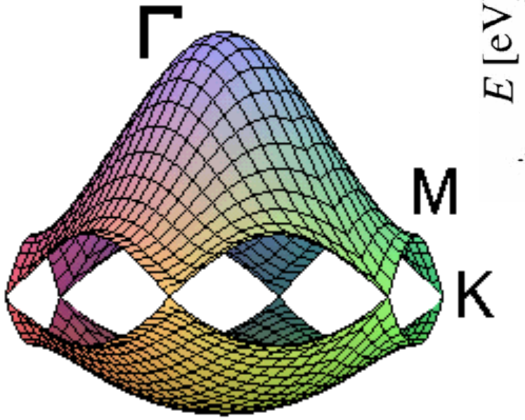


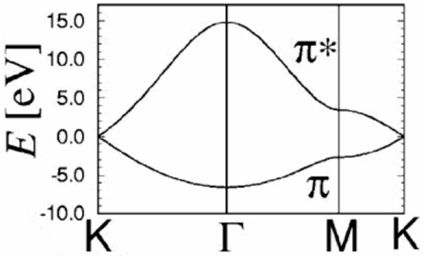


$$\mathbf{a}_1 = (\frac{\sqrt{3}}{2}, \frac{1}{2})a, \mathbf{a}_2 = (\frac{\sqrt{3}}{2}, -\frac{1}{2})a$$

$$\mathbf{b}_1 = (\frac{1}{2}, \frac{\sqrt{3}}{2})\frac{4\pi}{\sqrt{3}a}, \mathbf{b}_2 = (\frac{1}{2}, -\frac{\sqrt{3}}{2})\frac{4\pi}{\sqrt{3}a}$$

- Energy Band
  - Metal with zero gap

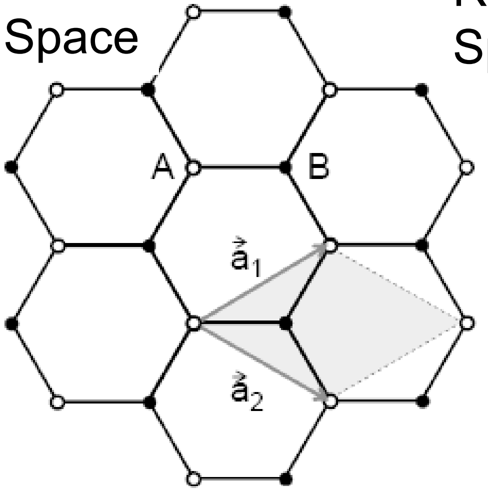


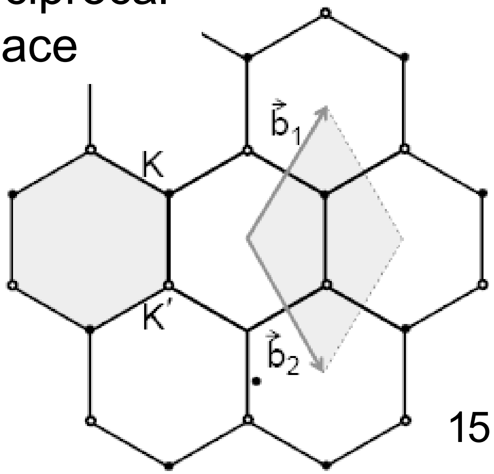


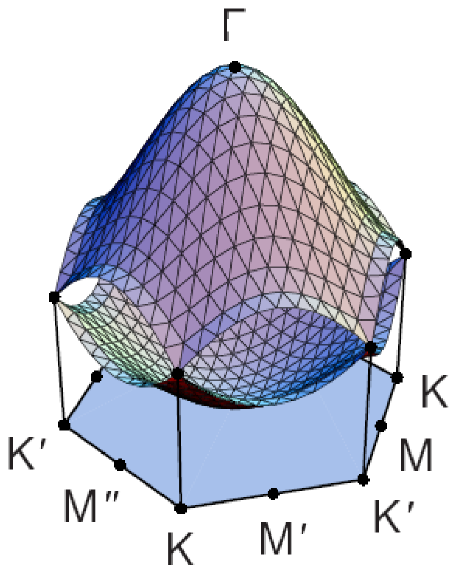
$$E_k = \pm t\sqrt{1 \pm 4\cos\frac{k_y a}{2}\cos\frac{\sqrt{3}k_x a}{2} + 4\cos^2\frac{k_y a}{2}}$$

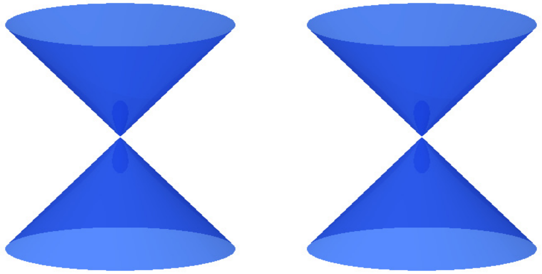
Twin Dirac Cones

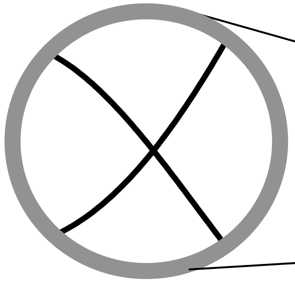
$$E = \sqrt{m^2c^4 + p^2c^2}$$

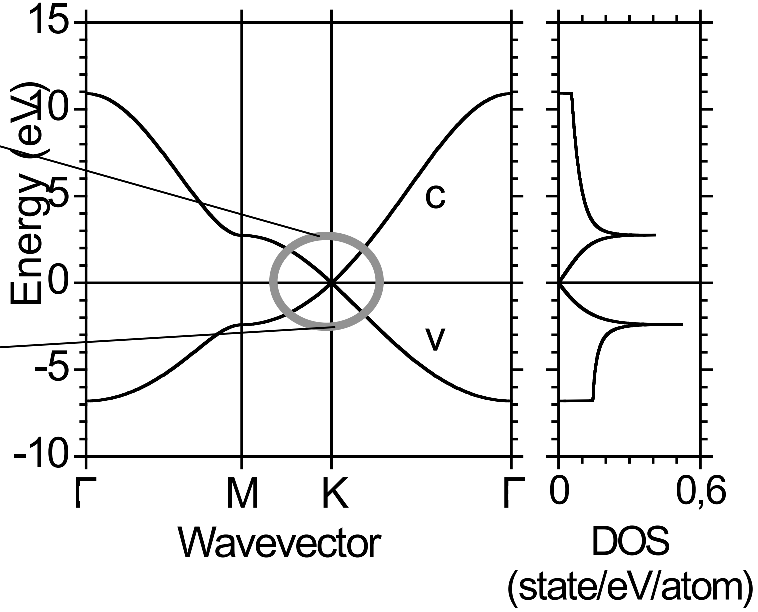

Real Space


Reciprocal Space



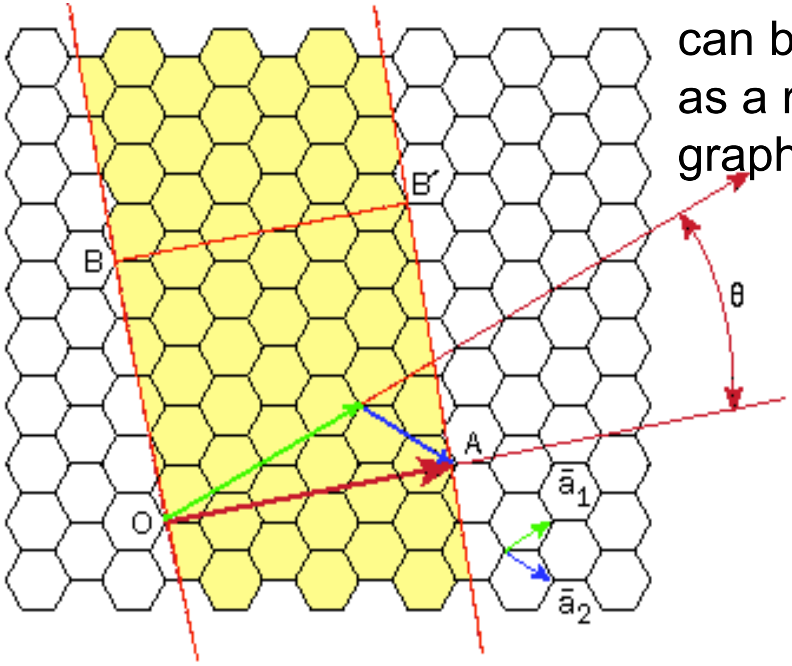






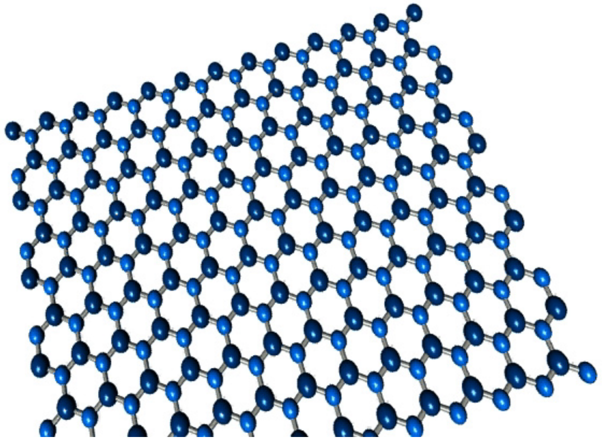
Graphene Physics
= Magic of Symmetry

Carbon Nanotubes

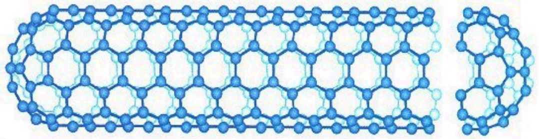


(**4**,**2**)

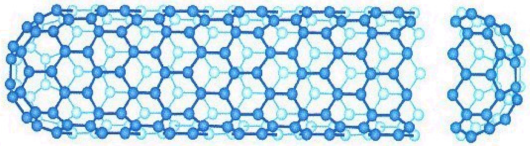
Carbon Nanotubes can be understood as a rolled-up graphene layer



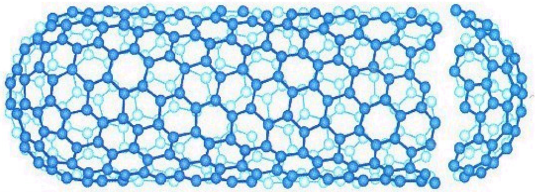
ARMCHAIR
$\theta = 30^\circ$



ZIGZAG
$\theta = 0^\circ$



CHIRAL
$0^\circ < \theta < 30^\circ$



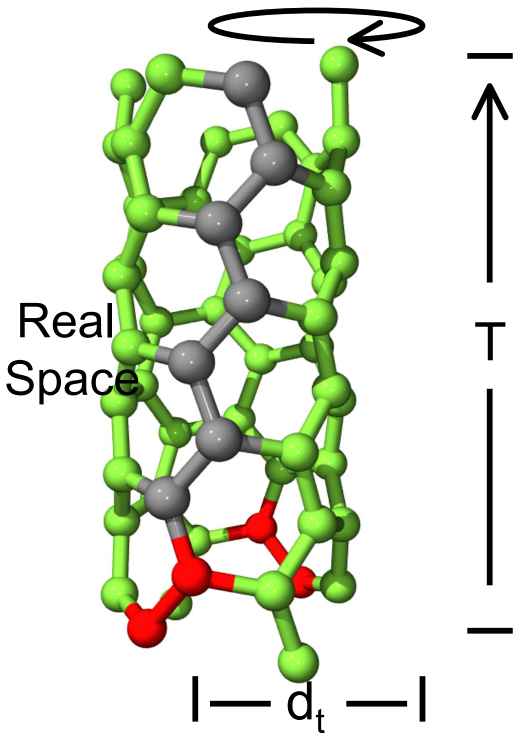
Diameter
$$d_t = \sqrt{3} a_{C-C} (n^2 + m^2 + nm)^{1/2} / \pi$$

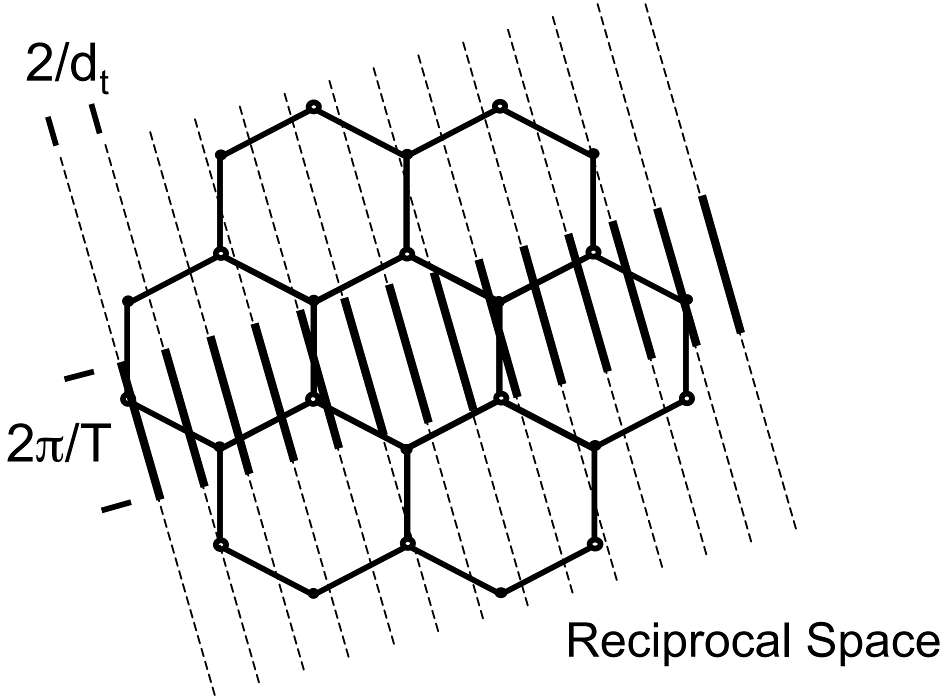
Chiral angle
$$\theta = \tan^{-1}\left(\frac{\sqrt{3} m}{2n + m}\right)$$

Recoprocal Lattice vectors of single wall carbon nanotubes

Confinement around nanotube circumference

Quantization of the angular momentum $\mu=2\pi/\pi d_t$



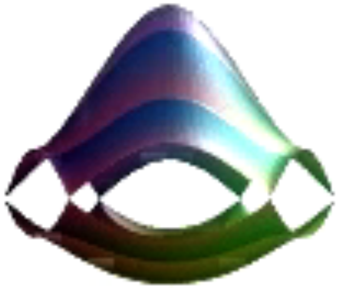


Periodic Boundary Condition along the nanotube axis

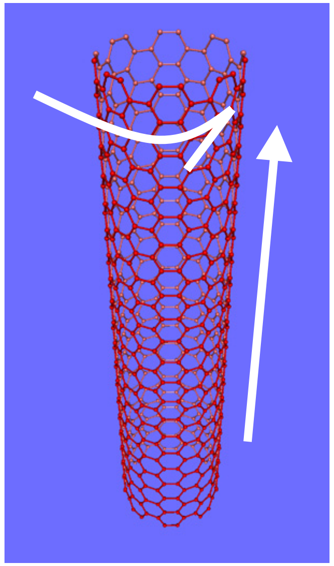
Definition of a 1D Brillouin zone of lenght $2\pi/T$

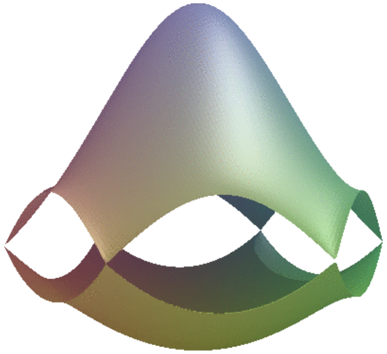
Brillouin zone of nanotubes

R. Saito *et al.*, *Phys. Rev*. **B46**, 1804 (1992)

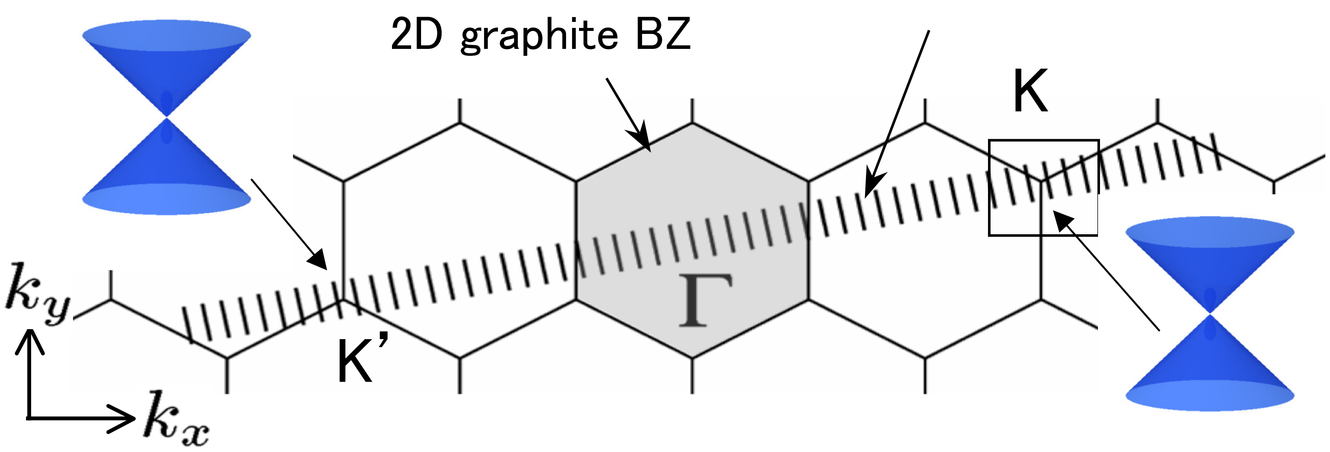


(C) Gleb Zhelezov





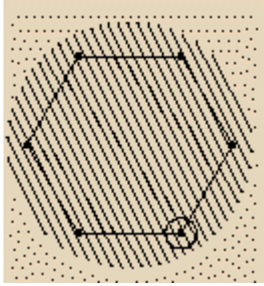
Brillouin zone (BZ)



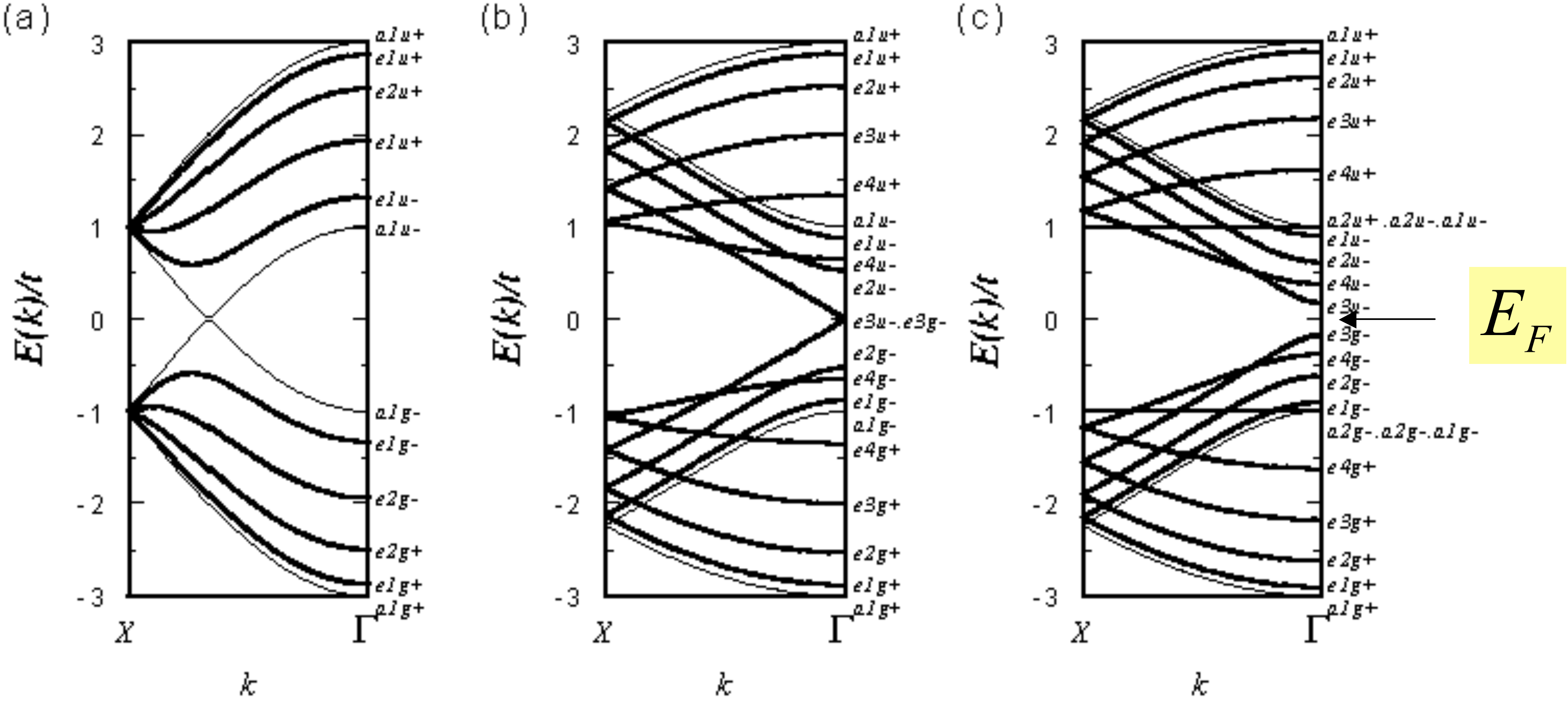
cutting lines = 1D Brillouin zone

Energy Bands of Nanotubes

R. Saito *et al.*, *Phys. Rev*. **B46**, 1804 (1992)



- *N* one-dimensional bands

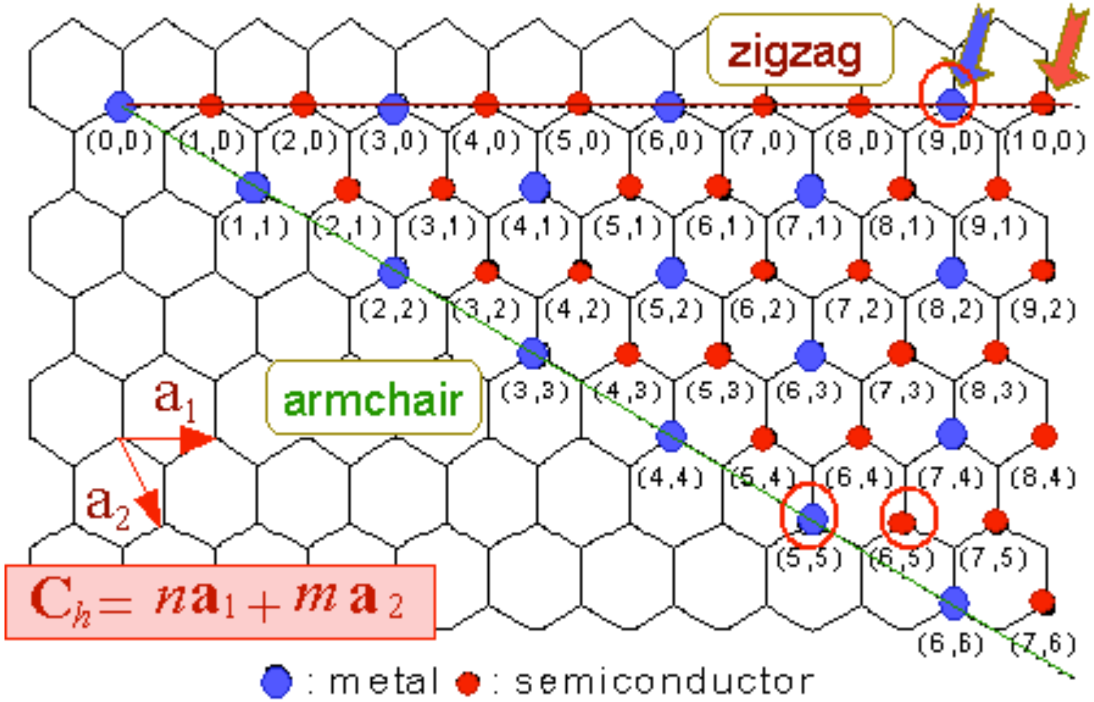


(5,5) (9,0) (10,0)

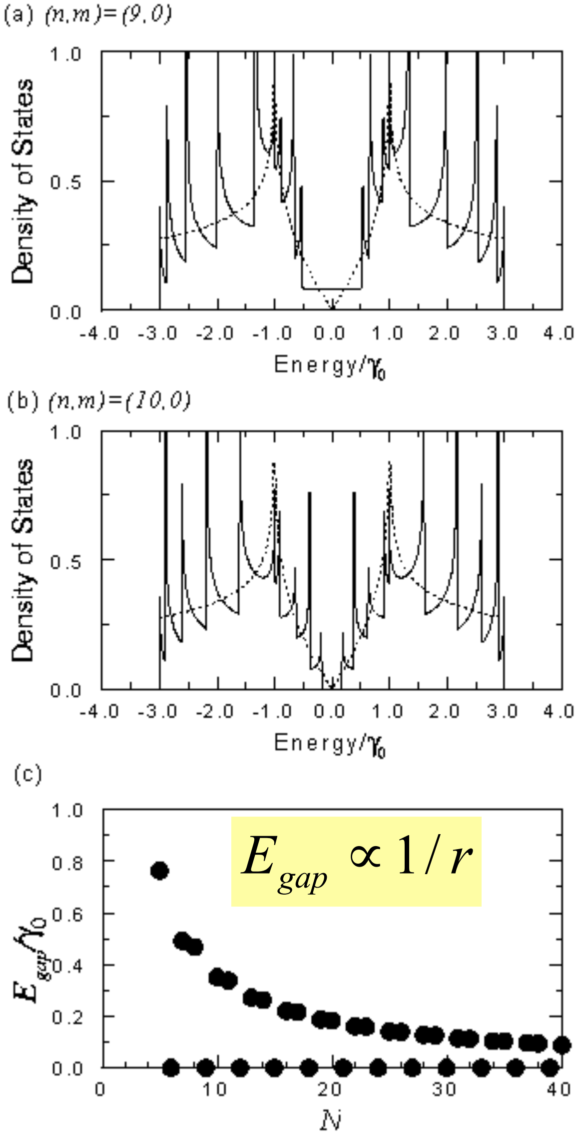
根据直径和手性不同纳米碳管可以表现为金属属性或半导体属性

- Density of States
- depending on chirality

R. Saito *et al., Appl. Phys. Lett.* **60**, 2204 (1992)

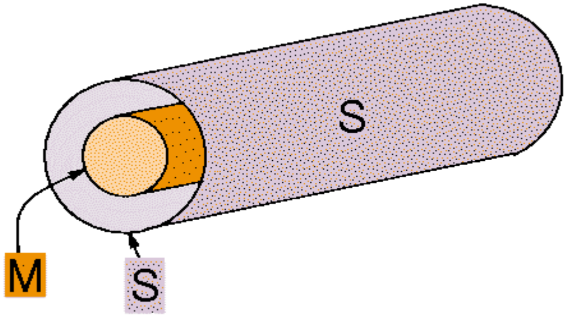


$$n-m=\begin{cases}3p & \text{metal}\\ 3p\pm1 & \text{semiconductor}\end{cases}$$

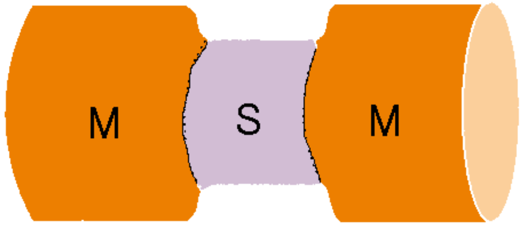


Semiconductor Devices

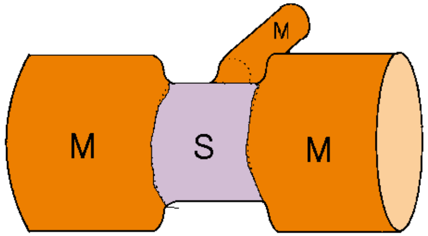
R. Saito *et al*. Proc. of the NEC Symp. (1992)



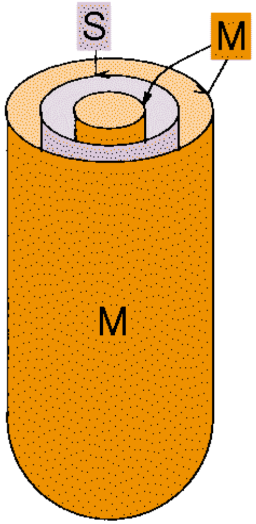
Metallic Wire



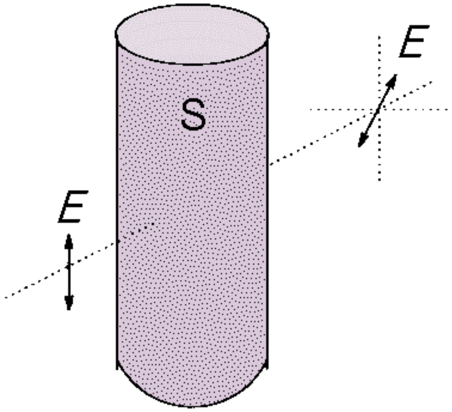
Junctions



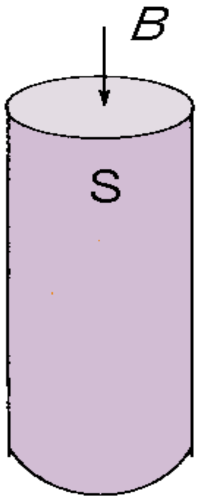
Logical Circuit



Memory



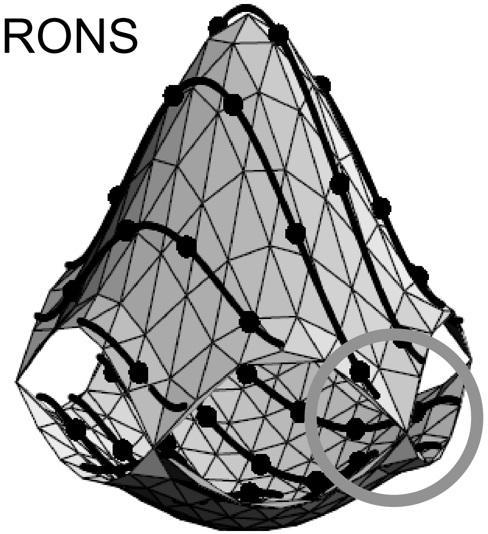
Optical Devices



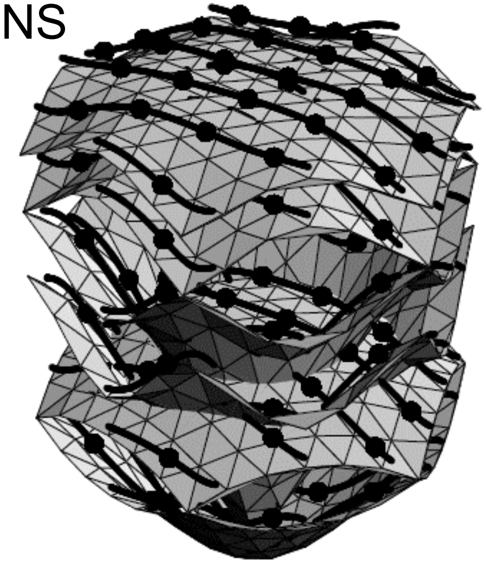
Magnetic Devices

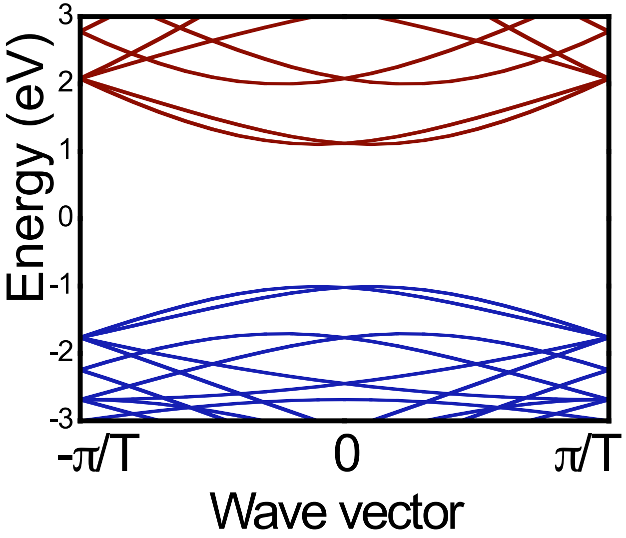
Mod(2n+m,3) = 0, 1, and 2

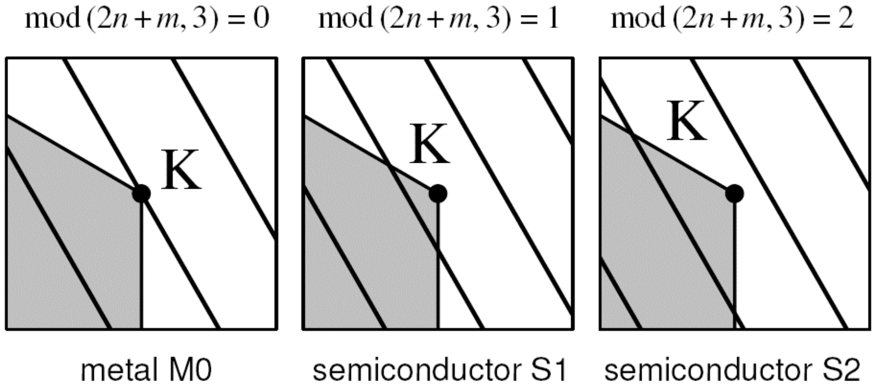
ELECTRONS



PHONONS

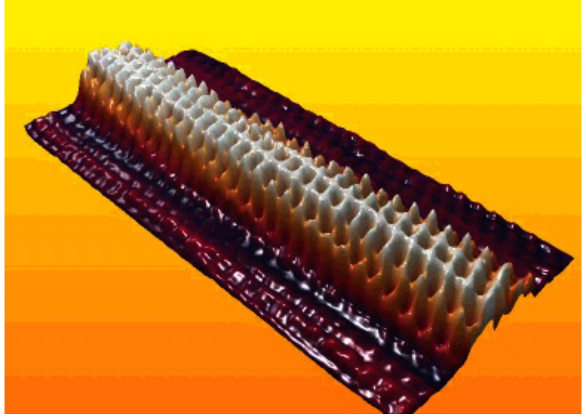




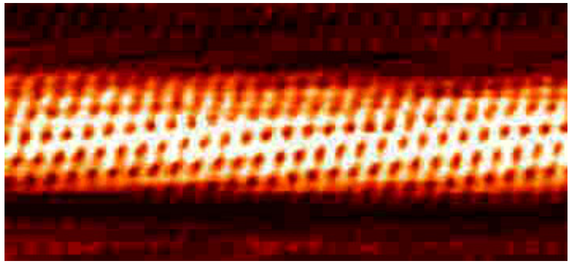


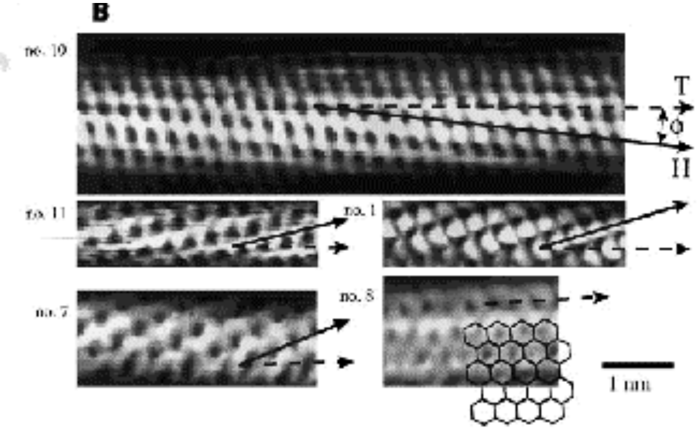
metal M0 semiconductor S1 semiconductor S2

Can be either metallic or Semiconducting

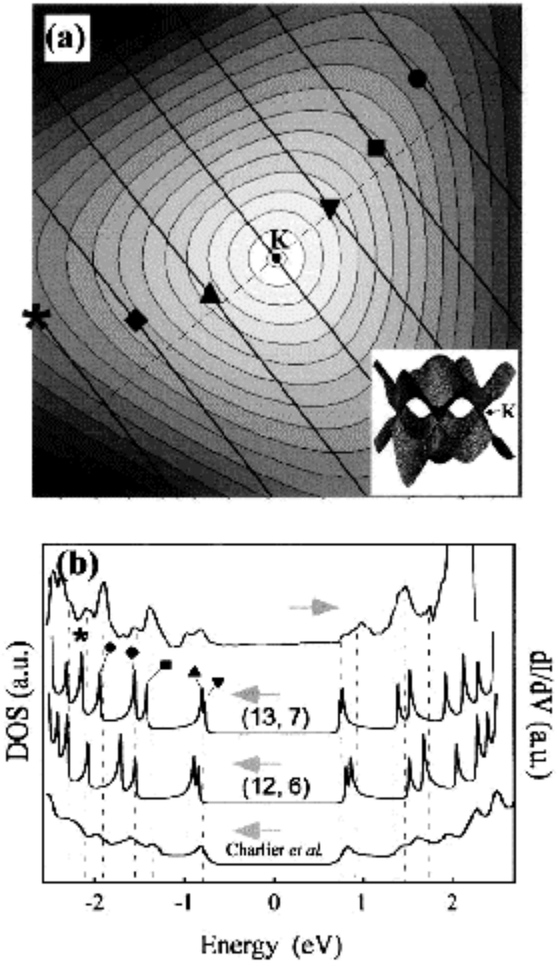


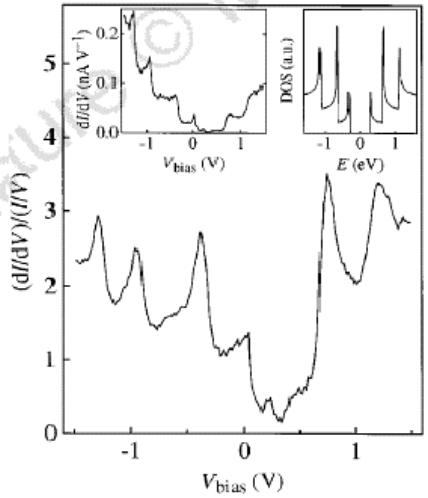
STM/STS
Experiments

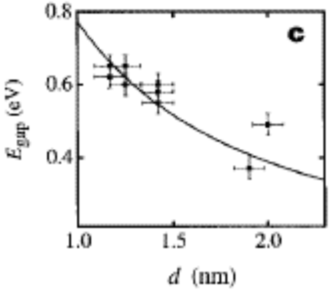




P. Kim et al., PRL 82, (1999) 1225.



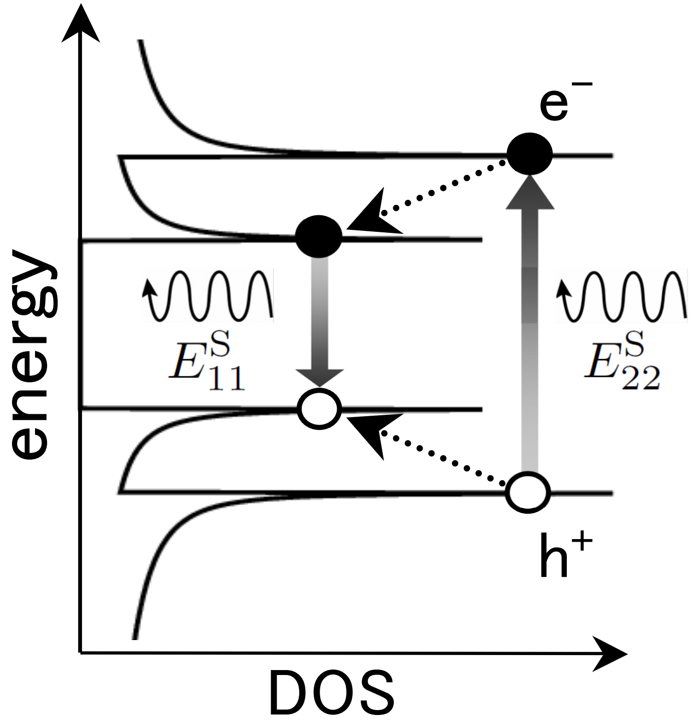




J. W. G. Wildoer et al, Nature, 391 (1998) 59

Photo-Luminescence (PL)

Optical Process of PL



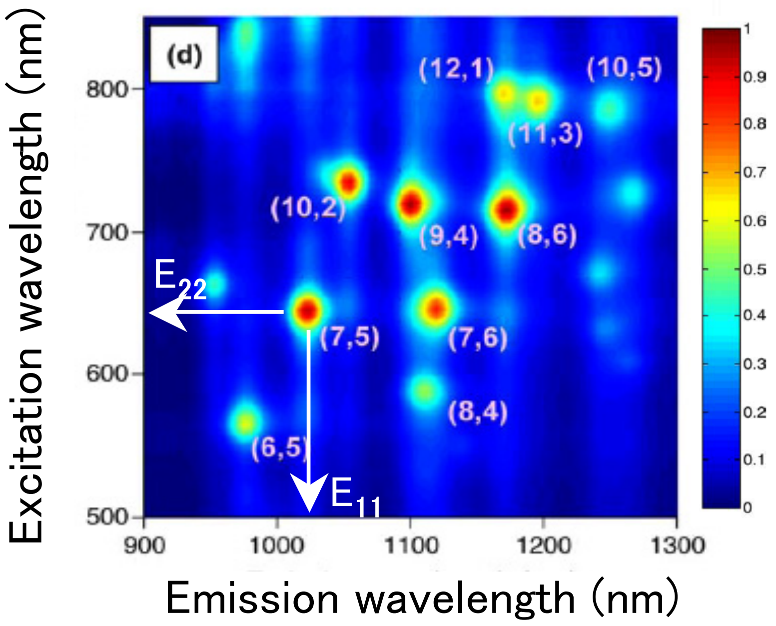
(1) photo absorption

(2) relaxation by phonon

(3) photo emission

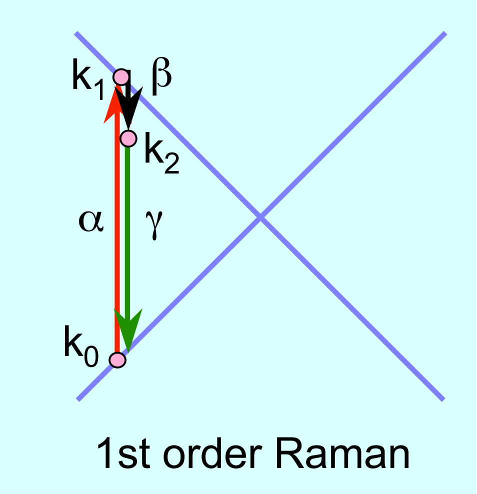
PL from diffrent (n,m)

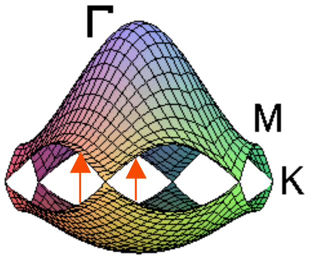
M. J. O’Connel *et al.*, Science **297**, 593 (2002)
S. M. Bachilo *et al.*, Science **298**, 2361 (2002)
Y. Miyauchi *et al.*, Chem. Phys. Lett. **387**, 198 (2004)

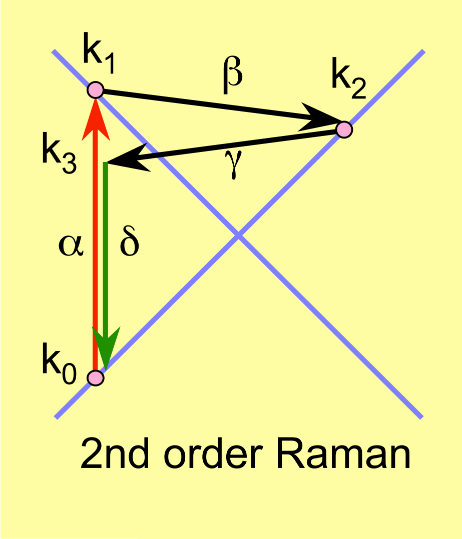


PL Intensity chirality dep.
type I - type II dep.

Resonance Raman Intensity







- 1st order Raman

Electron phonon interaction

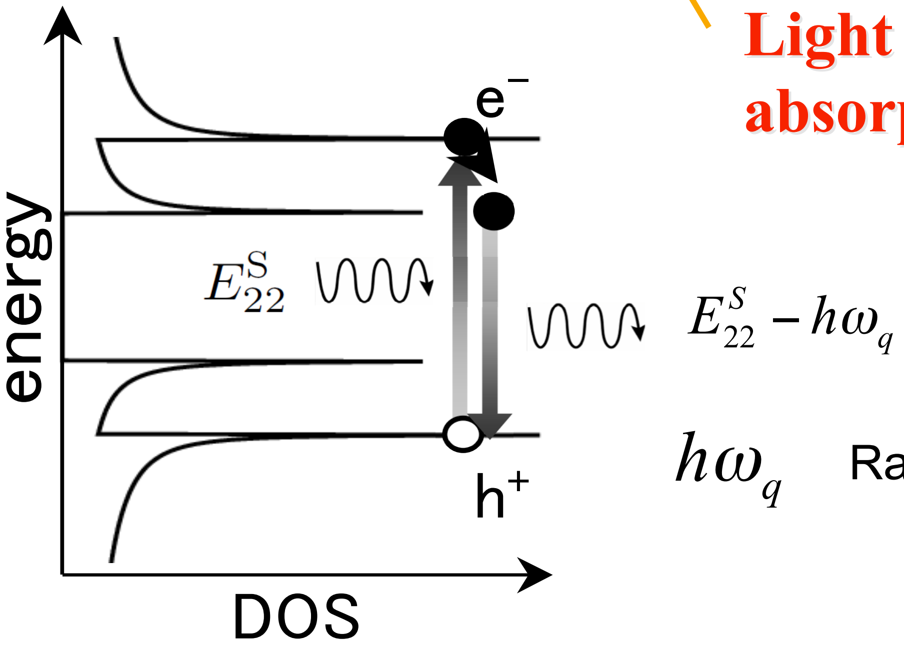
Light emission

Light absorption

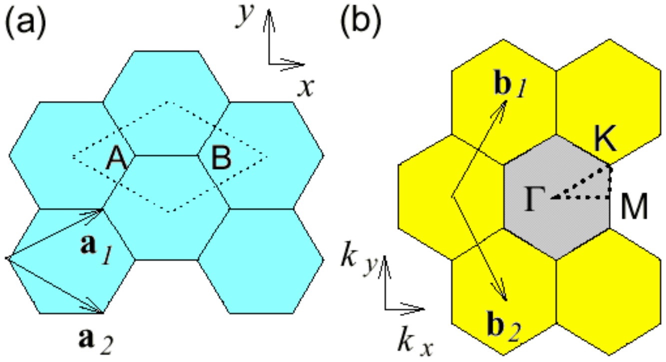
Intensity is enhanced

When optical absoption

occues.



Raman shift



Phonon Dispersion of 2D graphite

R. Saito et al., “Physical Properties of Carbon Nanotubes” Imperial College Press (1998)

Determination of phonon energy dispersion relation

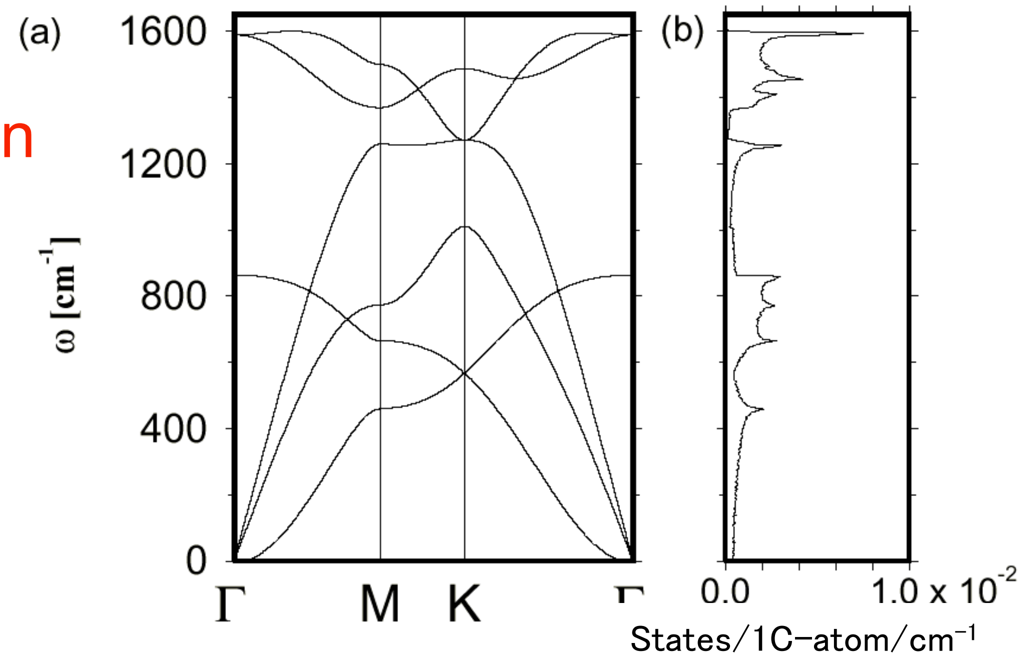
1. Inelastic neutron scattering
2. EELS
3. Double resonance Raman

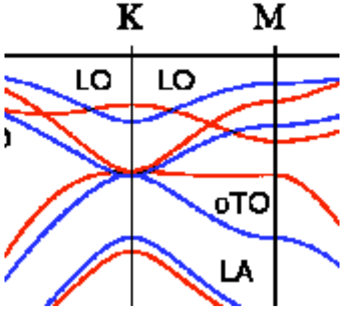
Special Merit of Raman:

Disordered material

Small quantity

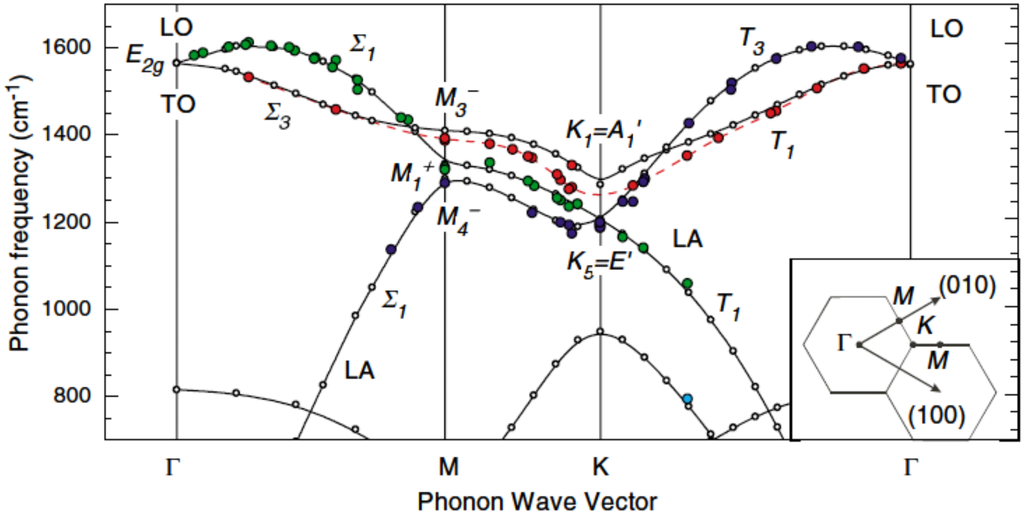
zone boundary





Phonon dispersion of graphite by inelastic X-ray

J. Maultzsch et al, *Phys. Rev. Lett.* 92, 075501 (2004)



high accuracy measurement around K point by 17kev X-ray

& ab initio calculation

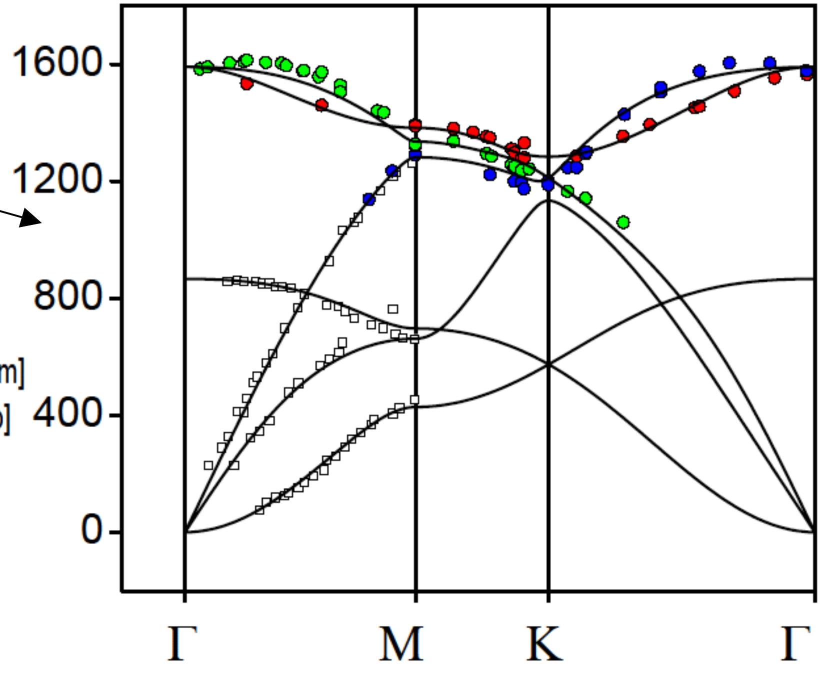
Force constant fitting by G. Ge. Samsonidze

slope 29cm^{-1}/eV (KM) 41cm^{-1}/eV (KΓ)
(53cm^{-1}/eV) PTW = 12cm^{-1} (24cm^{-1})

Four nearest-neighbor force-constant phonon dispersion of graphene layer [f.c. units – 10^{4}dyn/cm]
Colored dots – Maultzsch x-ray, open squares – Jishi neutron [initial set of f.c. – Dubay ab initio]

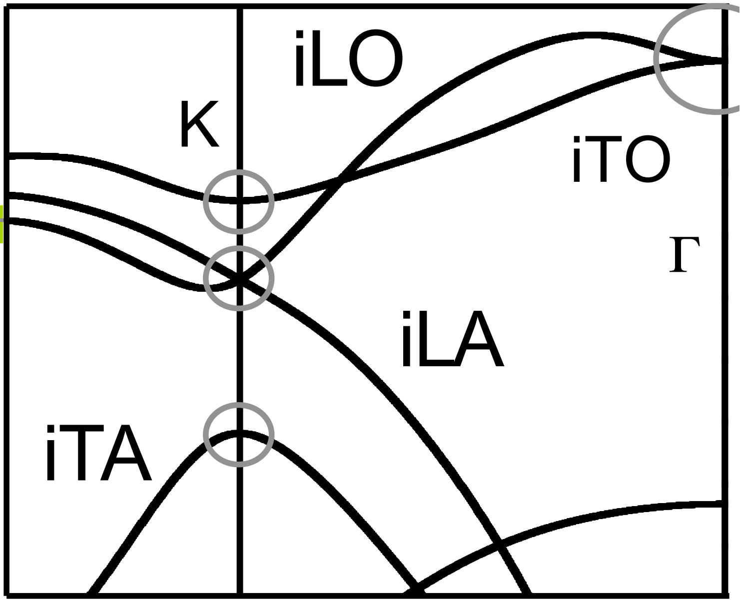
$\phi_r^1=+39.28$ $\phi_{ti}^1=+11.36$ $\phi_{to}^1=+10.18$ $\phi_r^3=-6.14$ $\phi_{ti}^3=+9.27$ $\phi_{to}^3=-0.46$

$\phi_r^2=+6.34$ $\phi_{ti}^2=-3.18$ $\phi_{to}^2=-0.36$ $\phi_r^4=+2.53$ $\phi_{ti}^4=+0.40$ $\phi_{to}^4=-0.44$

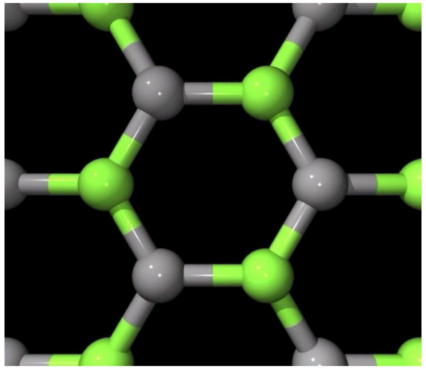


Graphite

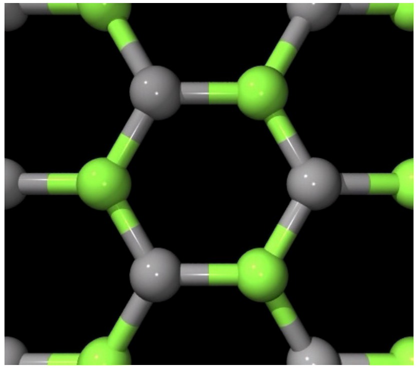
Vibrational Properties



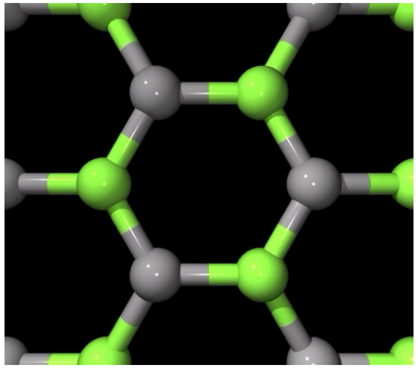
Γ - iLO



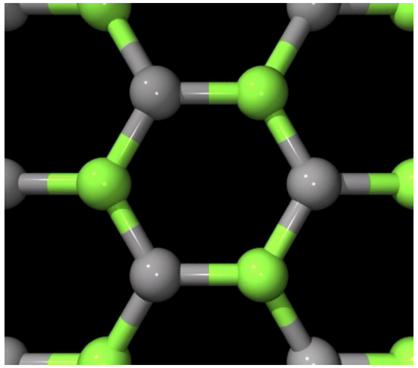
Γ - iTO



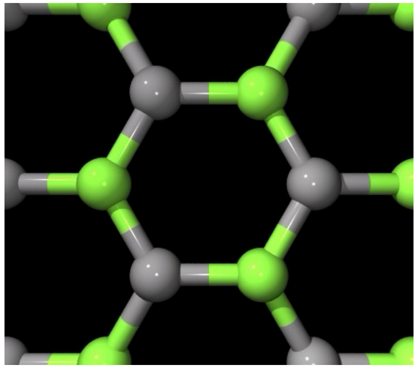
K - iTO



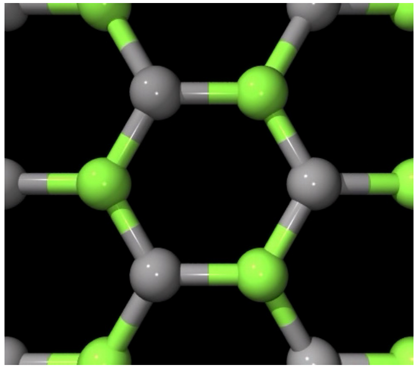
K - iLO



K - iLA



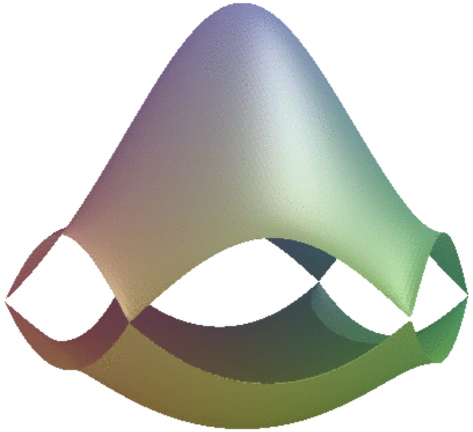
K - iTA

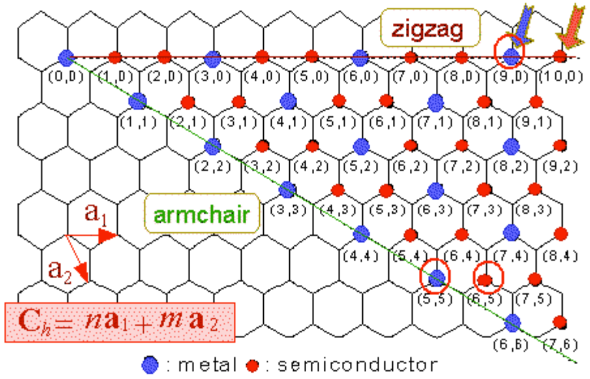


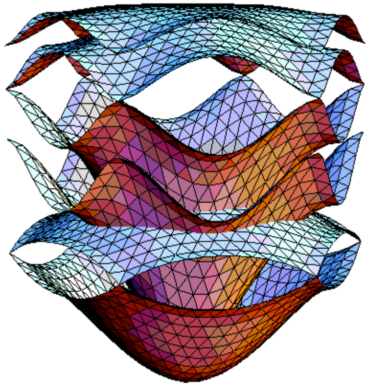
Courtesy of Dr. Ge. G. Samsonidze

Summary :electron and phonon of nanotubes

- Structure is determined by (n,m)
- Electronic structure of a SWNT
  - 1D energy subband (cutting lines)
  - Metal or semiconductor
  - density of states (van Hove singularity)
- Phonon structure of a SWNT (graphene)
  - 6 phonon modes LA 2 iTA oTO LO TO

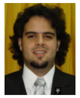


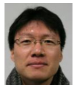




Intensity calculation of PL and Raman spectra
-- *Not all SWNTs are bright.* --

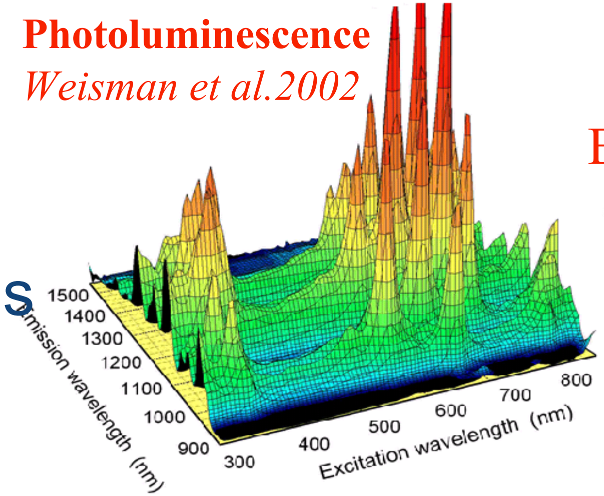
- PL and Raman intensity
  - (n,m) dependence
  - RBM,G, D, G'-band
  - (n,m) population analysis
  - Length dependence
  - Pressure dependence
  - exciton based phenomena





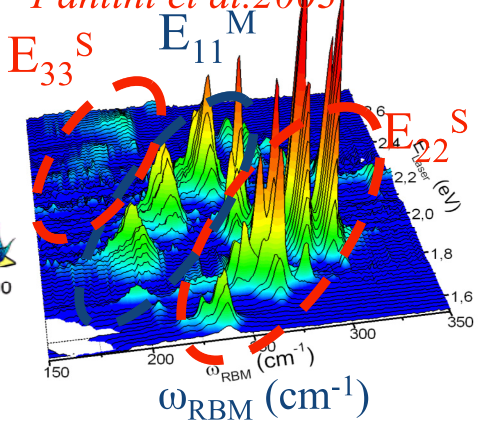
Photoluminescence

Weisman et al.2002



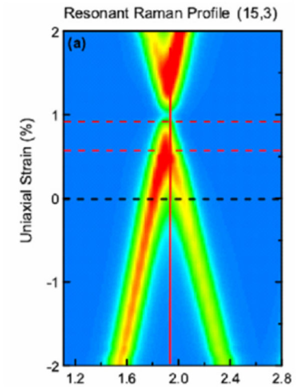
Resonance Raman

Fantini et al.2003



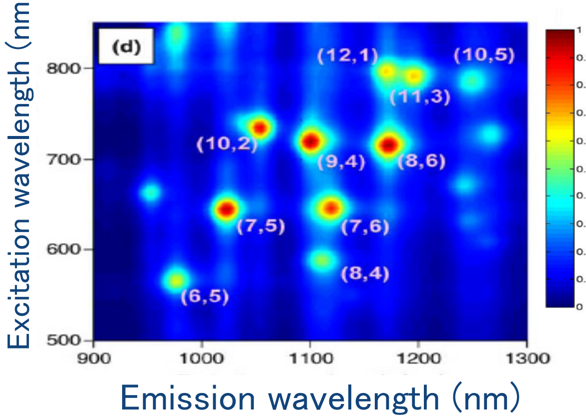
Pressure dependent Raman

A. Souza-Filho et al.2006



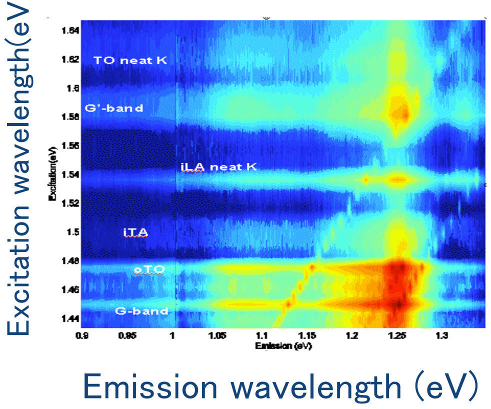
Type dependent PL

Maruyama et al.2004



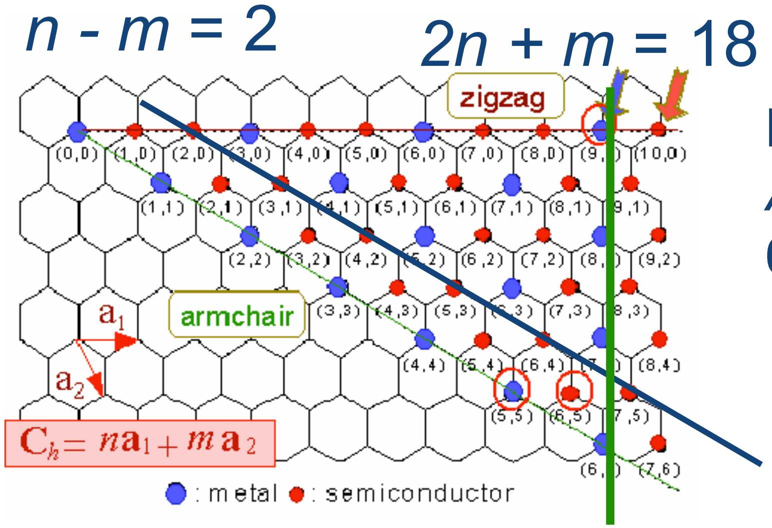
Phonon associated PL

S. G. Chou et al.2005

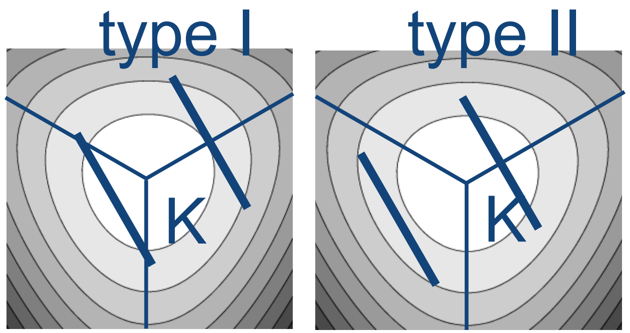


2n+m and *n−m* family in SWNT

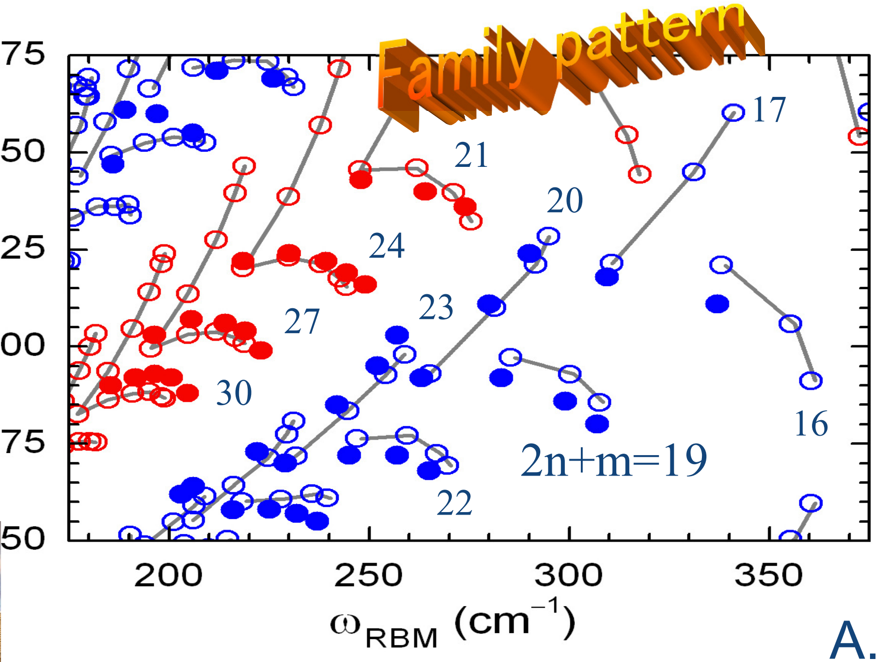
R. Saito *et al*., *Phys. Rev*. B, 72, 153413 (2005)

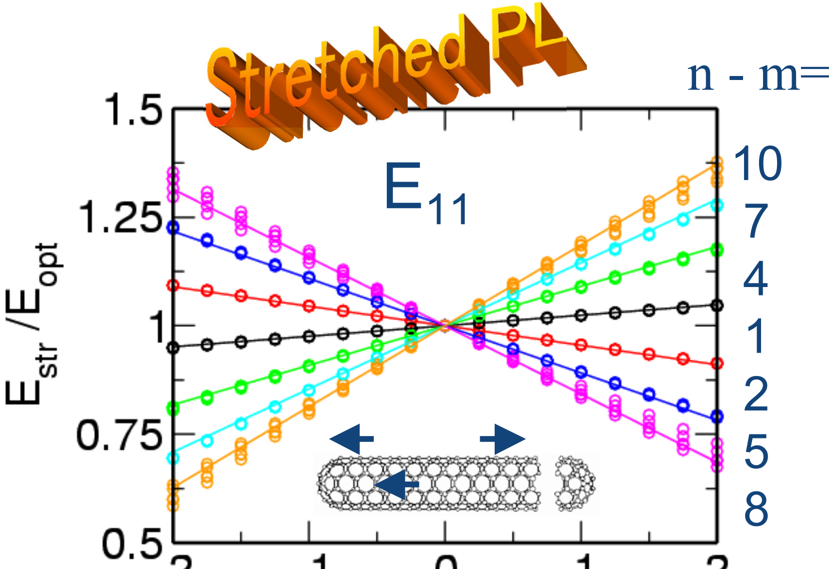


R. Saito *et al*., *Appl. Phys. Lett.* **60**, 2204 (1992)



	type I	type II
$\mathrm{mod}\,(2n+m,3) =$	1	2
$\mathrm{mod}\,(n-m,3) =$	2	1



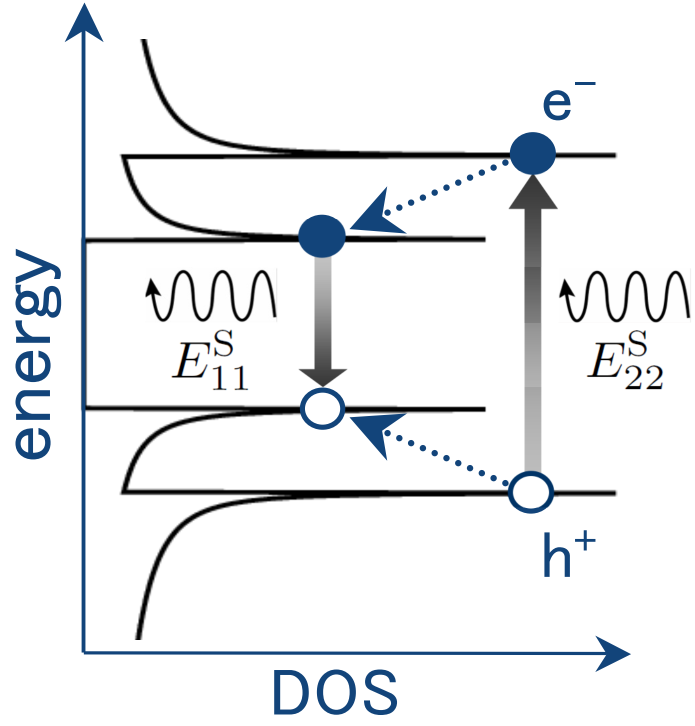


A. G. Souza-Filho et al., PRL (2006)

Photo-Luminescence (PL)

Y. Oyama *et al, Carbon*, 44, 873 (2006)

Optical Process of PL



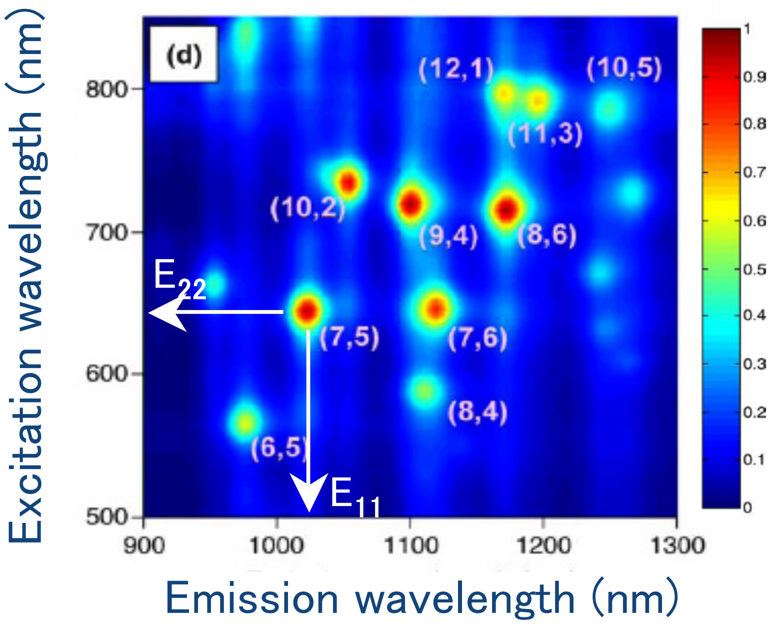
(1) photo absorption

(2) relaxation by phonon

(3) photo emission

PL from diffrent (n,m)

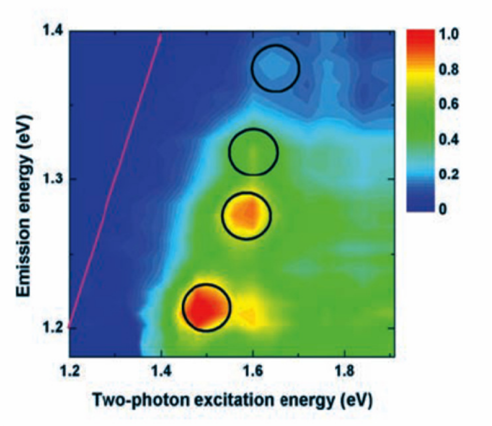
M. J. O' Connel *et al.*, Science **297**, 593 (2002)
S. M. Bachilo *et al.*, Science **298**, 2361 (2002)
Y. Miyauchi *et al.*, Chem. Phys. Lett. **387**, 198 (2004)



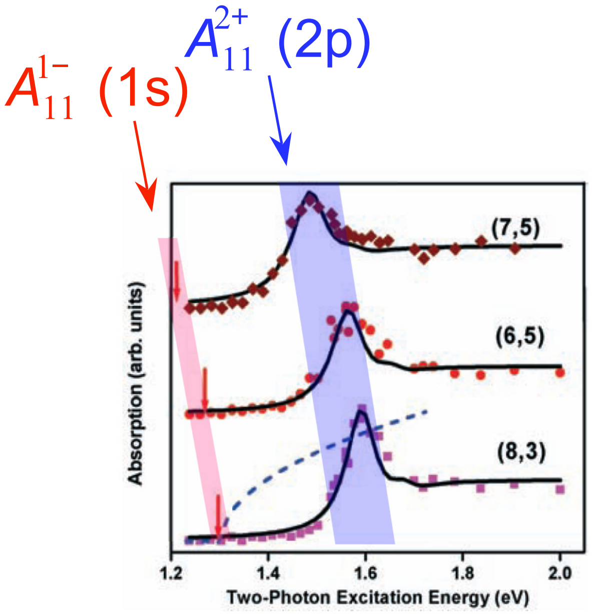
PL Intensity chirality dep.
type I - type II dep.

Exciton calculation

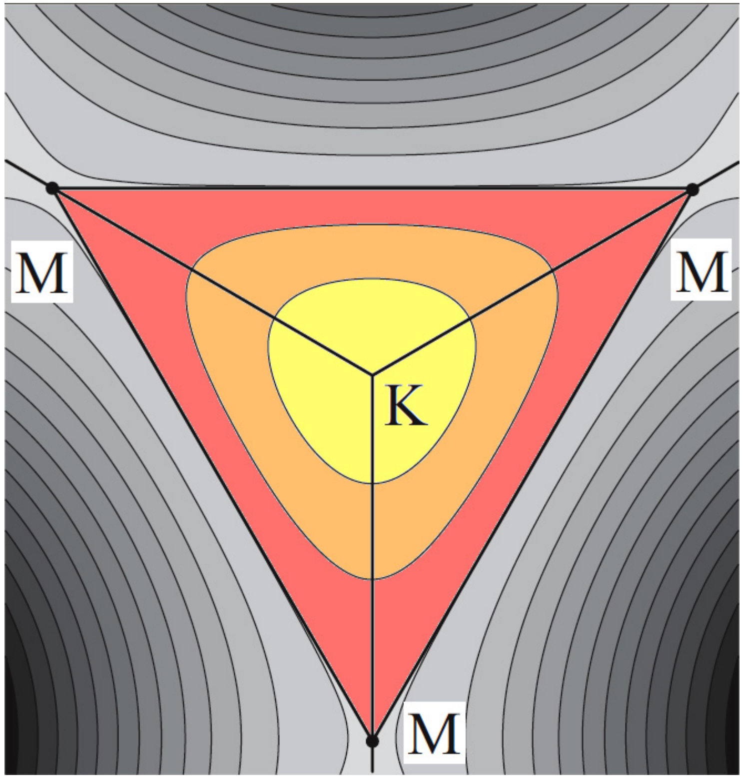
- Why?
  - Large binding energy (0.5eV)
    - even room temperature, exciton exists.
  - Exciton specific phenomena
    - dark exciton, two photon, environment
- What can we imagine?
  - Localized exciton wave function
    - enhancement of optical process
    - Direct energy gap
    - Infrared energy region, tunable
- What is the problem?
  - Low quantum efficiency.

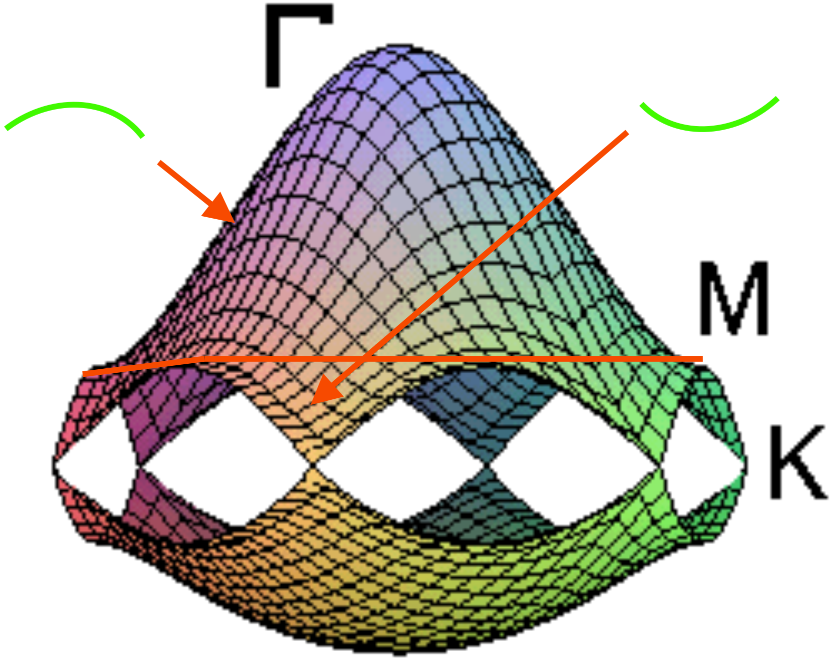


Wang et al. Science ***308**, 838 (2005)*



Exciton exists only in the 3M-triangle



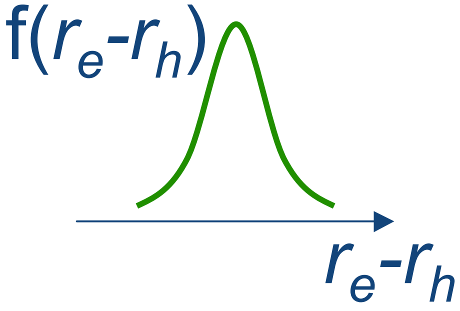


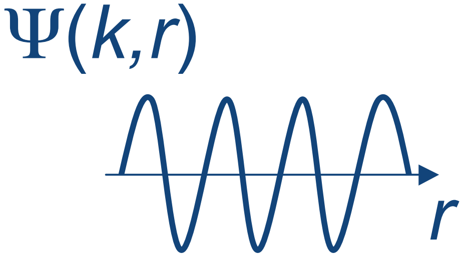
Energy minimum for the $\pi*$ band exists only in 3MΔ.

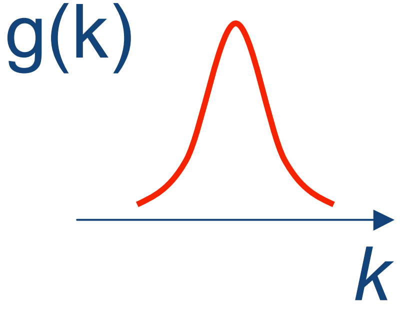
Energy maximum does not contribute to optical transition

For each (n,m), the highest *Eii* exists.

Exciton is localized in *r* and *k* space







- electron(e) – hole(h)
  - Coulomb interaction
- Exciton wavefunction $f(r_e - r_h)$ is localized in the real space
- In solid, Bloch wavefunction with k, $\Psi(k,r)$ delocalized
- Some $\Psi(k,r)$'s are mixed by $g(k)$ to make the localized $f(r_e - r_h)$.
- How? the Bethe-Salpeter Eq.

ETB extension for Exciton

J. Jiang et al. *Phys. Rev.* B75 035405 and 035407(2007)

Bethe-Salpeter Equation

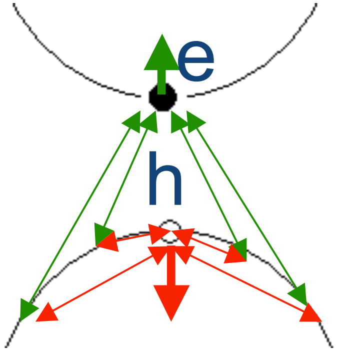
C. D. Spataru et al. PRL ***92,*** *077402 (2004)*

$$\left[(E_{k_c}-E_{k_v})\delta_{k_c k_{c'}}\delta_{k_v k_{v'}} + K_{k_c k_v, k_{c'} k_{v'}}\right]\Psi^n_{k_{c'}k_{v'}} = \Omega_n \Psi^n_{k_c k_v}$$

quasi-particle (QP) energy   Coulomb interaction (C)

$$K_{k_c k_v,k_{c'}k_{v'}} = 2\delta_S K^x_{k_c k_v,k_{c'}k_{v'}} + K^d_{k_c k_v,k_{c'}k_{v'}}$$

exchange C   direct C



Self-energy (Coulomb repulsion)

T. Ando J. Phys. Soc. Japan, ***66****, 1066 (1997),*

$v(\mathbf{r},\mathbf{r}')$ Ohno's potential / κ static dielectric constant to consider polarization of environment

RPA approximation: $V(\mathbf{q}) = v(\mathbf{q})/\epsilon(\mathbf{q})$ $\epsilon(\mathbf{q}) = 1+\frac{v(\mathbf{q})}{V}\Pi(\mathbf{q})$

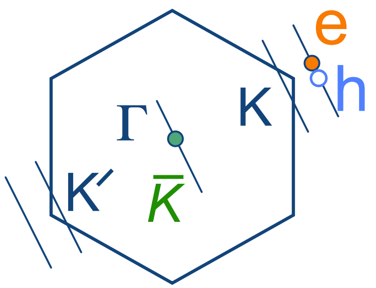
$$\Pi(\mathbf{q}) = -2\sum_{k,l,l'} \frac{f_{\mathbf{k}+\mathbf{q},l'}-f_{\mathbf{k},l}}{\epsilon_{\mathbf{k}+\mathbf{q},l'}-\epsilon_{\mathbf{k},l}} \left| <\mathbf{k}l|e^{-i\mathbf{q}\cdot\mathbf{r}}|\mathbf{k}+\mathbf{q},l'> \right|^2$$

$$\mathrm{E}_{kv} = \sum_q \sum_{sus'u'} \frac{V_{sus'u'}}{\varepsilon(q)} e^{iq(Rus-Ru's')} C^*_{kv}(s) C_{k+q,v}(s) C^*_{k+q,v}(s) C_{kv}(s)$$

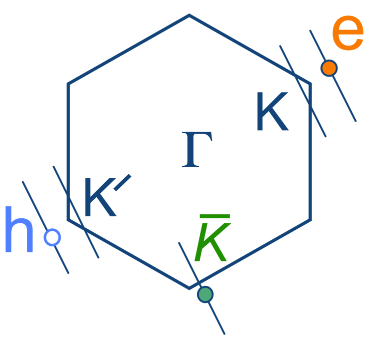
Symmetry of Excitons

J. Jiang et al. *Phys. Rev.* B75 035405 and 035407(2007)

A exciton



E exciton



not vertical transition

Center of mass $\overline{K} = k_e - k_h$

Relative motion $k = (k_e + k_h)/2$

A^- : bright exciton

A^+, E and E^*: dark excitons

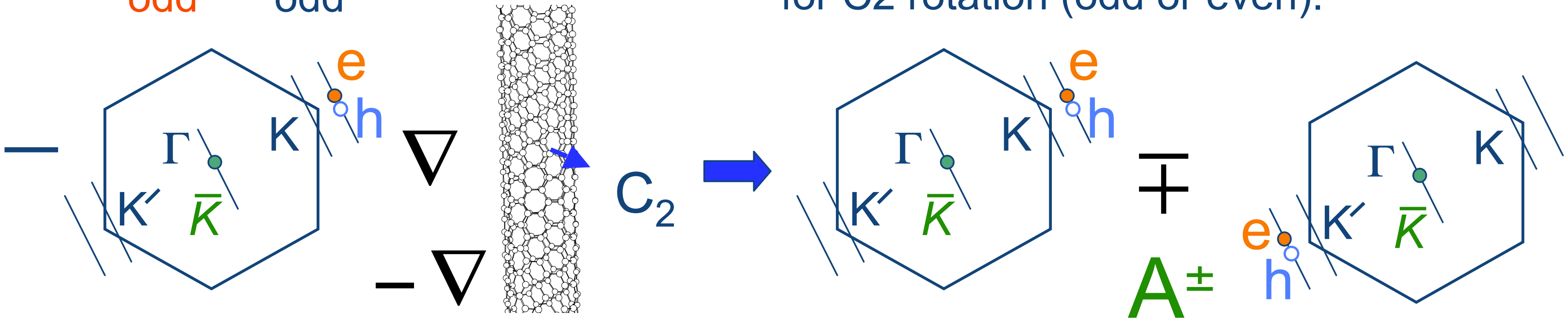
dipole transition matrix

$$\langle \Psi_{\text{exciton}} | \nabla | 0 \rangle \neq 0$$

odd odd

Bright and dark exciton

Eigen states are irreducible representation for C2 rotation (odd or even).



A+ even A- odd

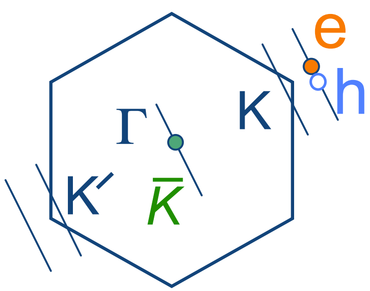
C_2 rotation for nanotube

J. Jiang et al. *Phys. Rev.* B75 035405 and 035407(2007)

dipole transition matrix

$$\left\langle \Psi_{\text{exciton}} \middle| \nabla \middle| 0 \right\rangle \neq 0$$

odd odd

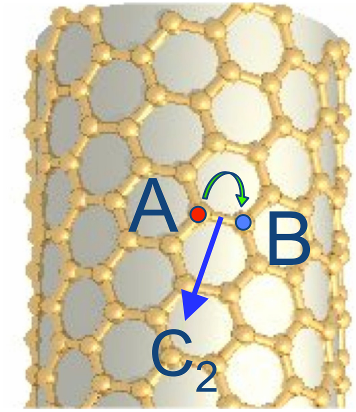


$$= C^{+}_{kc} C_{kv}$$

valence and conduction bands

$$\Psi_{\mathrm{v}}(k,r) = c^{A}_{\mathrm{v}}(k)\Phi^{A}_{\mathrm{v}}(k,r) + c^{B}_{\mathrm{v}}(k)\Phi^{B}_{\mathrm{v}}(k,r)$$

$$\Psi_{\mathrm{c}}(k,r) = c^{\mathrm{A}}_{\mathrm{c}}(k)\Phi^{\mathrm{A}}_{\mathrm{c}}(k,r) - c^{\mathrm{B}}_{\mathrm{c}}(k)\Phi^{\mathrm{B}}_{\mathrm{c}}(k,r)$$

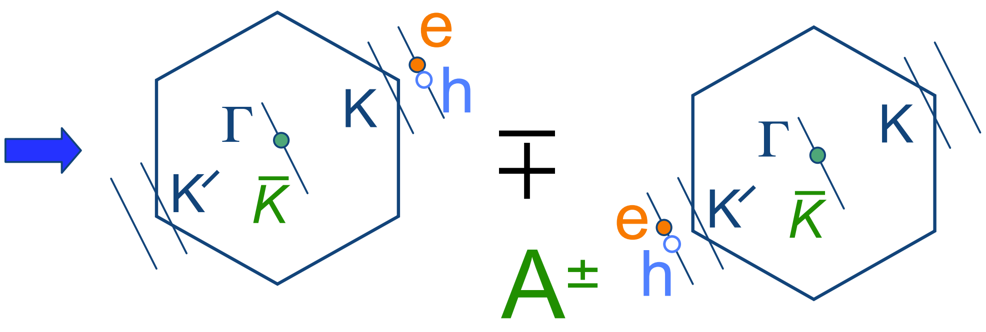


by C_2 rotation

$$k \to -k, \quad K \to K', \quad \mathrm{A} \leftrightarrow \mathrm{B}$$

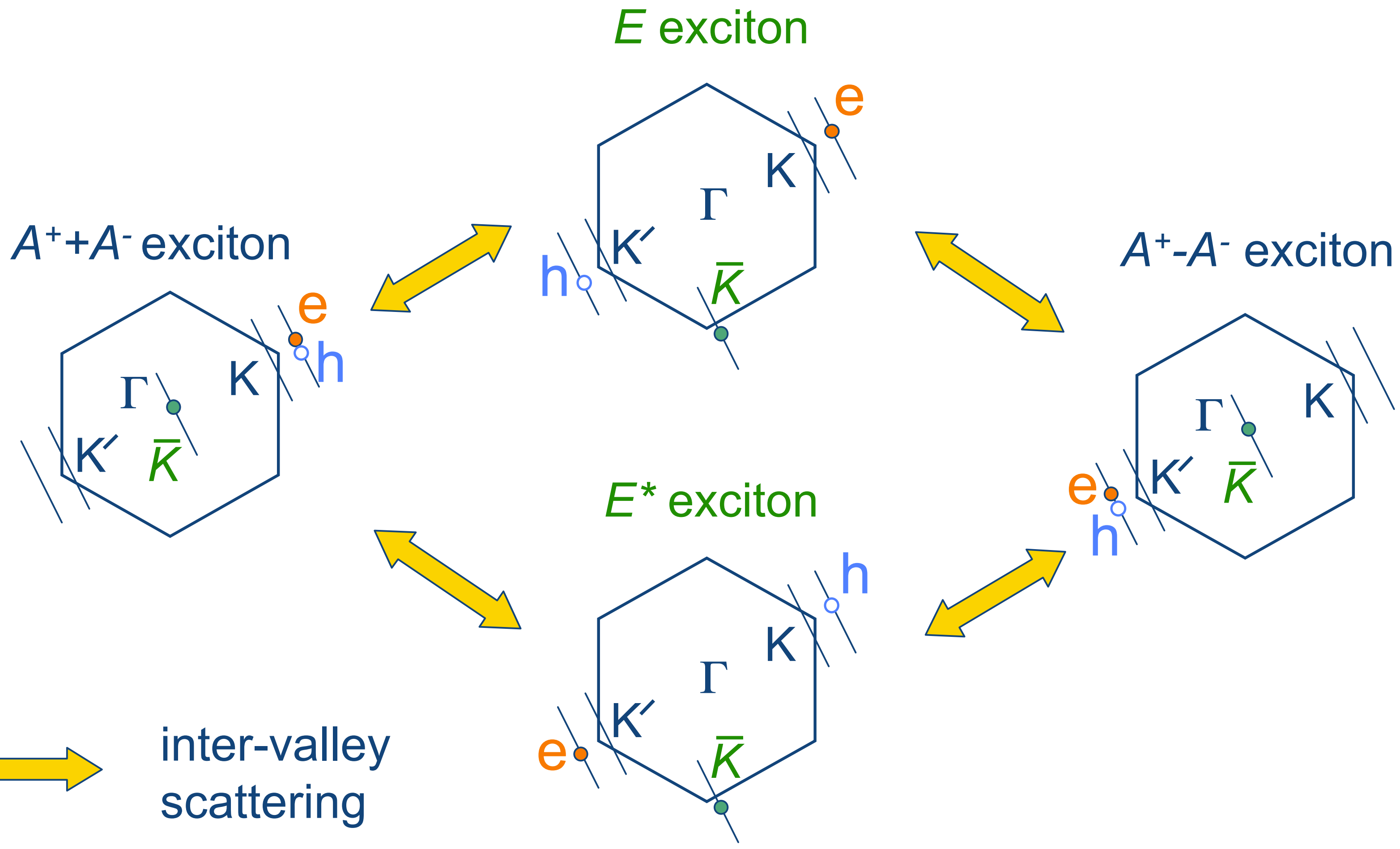
$$\Psi_{\mathrm{v}}(k,r) \to \Psi_{\mathrm{v}}(-k,r)$$

$$\Psi_{\mathrm{c}}(k,r) \to -\Psi_{\mathrm{c}}(-k,r)$$



A+ even A- odd

exciton-phonon interaction
- breaking symmetry -



⟷ inter-valley scattering

(fast!)

D-band, G’-band

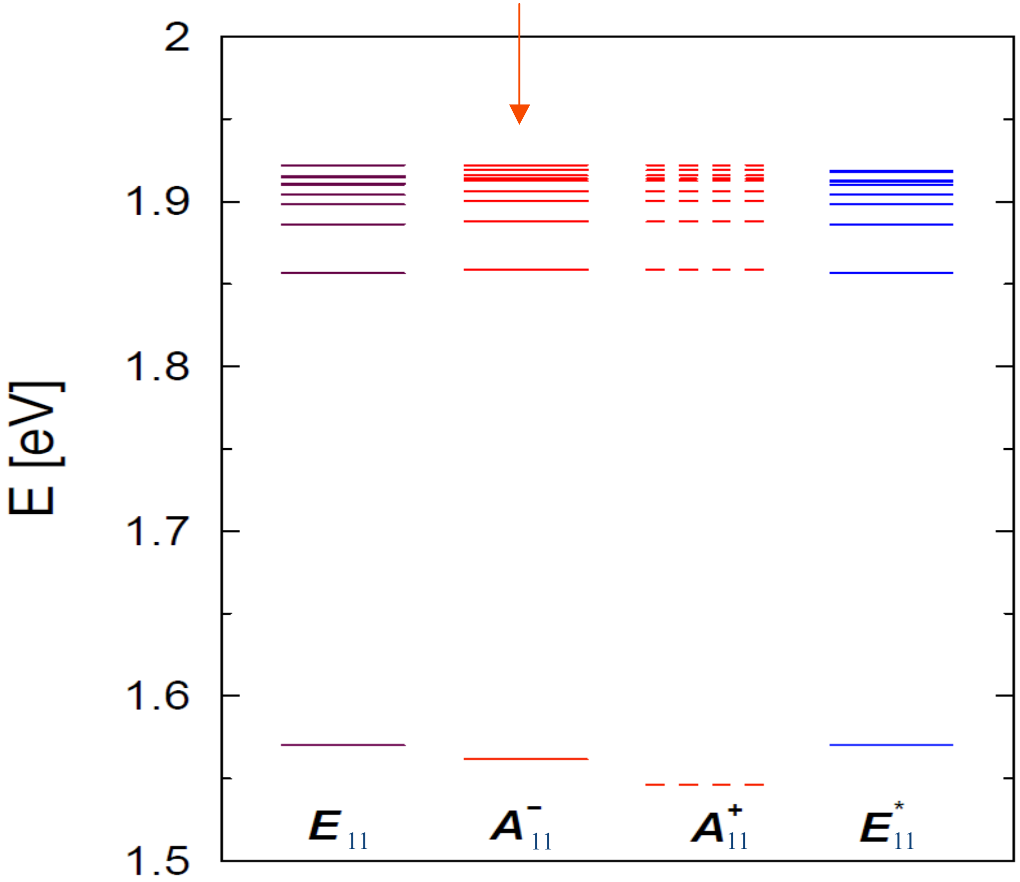
A^- : bright exciton

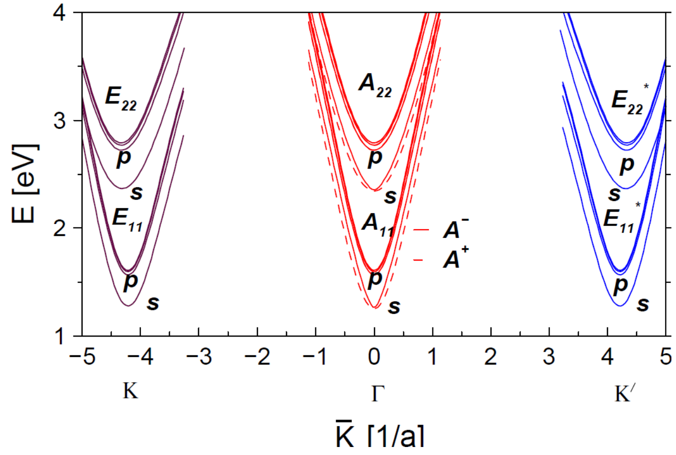
A^+, E, E^*: dark excitons

Dark state is the lowest

J. Jiang et al. *Phys. Rev.* B75 035405 and 035407(2007)

A^- : bright exciton (hereafter we only consider this)





Dispersion for (6,5) NT

A- : bright exciton

A^+, E and E^*: dark excitons

Double resonance Raman

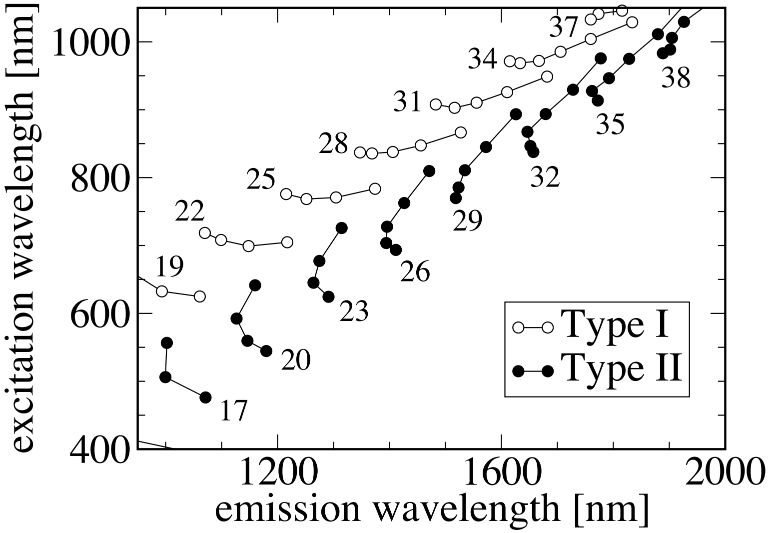
lowest but not allowed

Photoluminescence

Visible spectrum

E_{22}^{S}

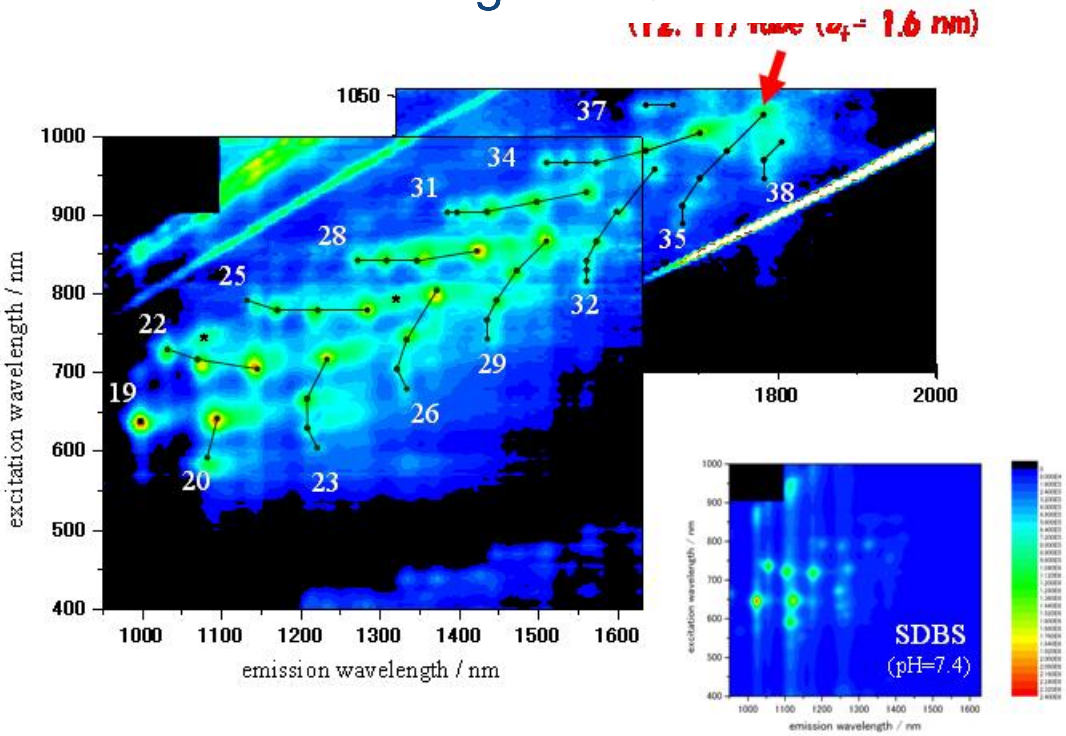
Calculation (κ=2.22)



E_{11}^{S}

experiment

PL from as-grown SWNTs



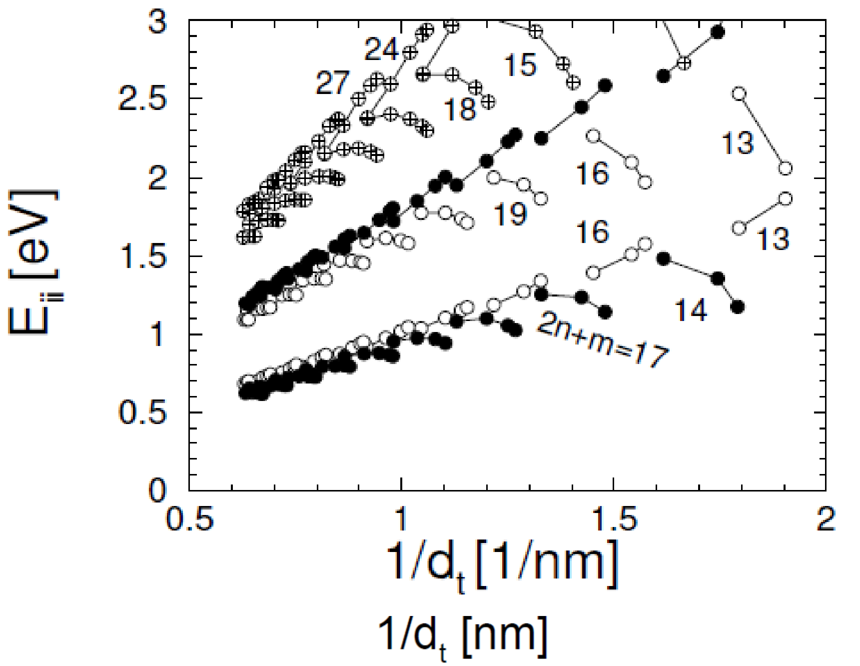
Dr. Toshiya Okazaki (AIST)

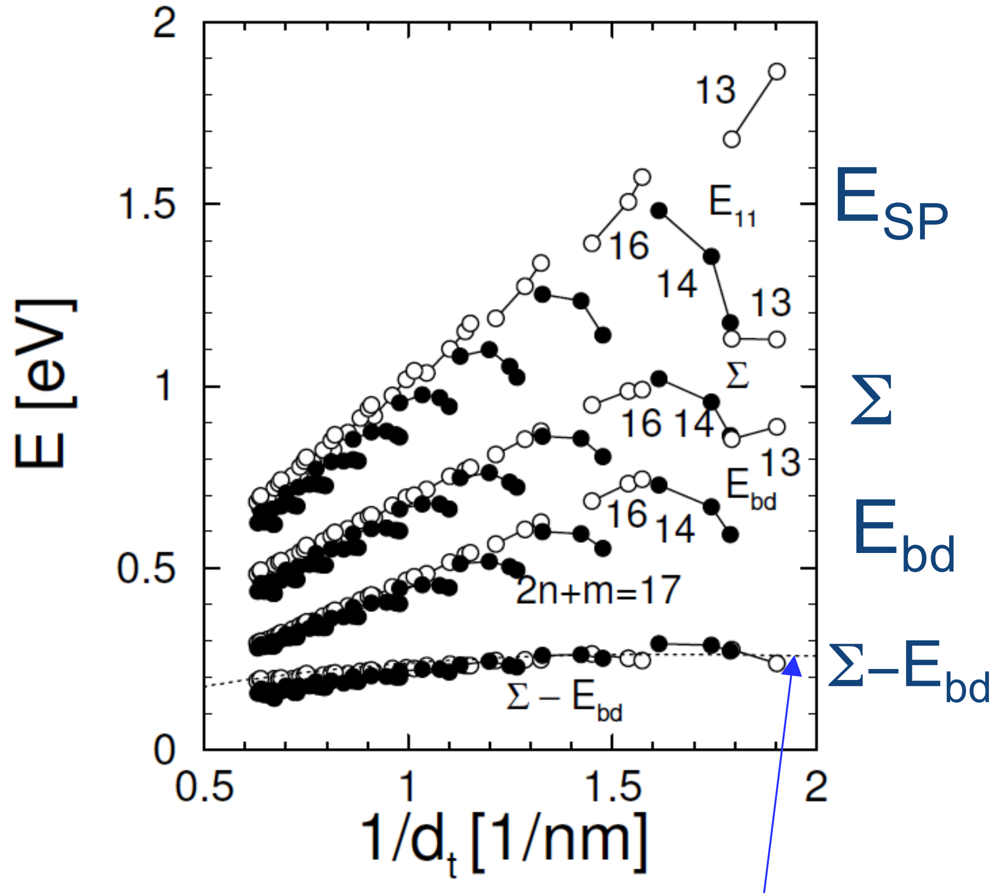
Some differences come from environmental effect around nanotubes

⇒ Optimizing the dielectric constant κ=2.22

Bright exciton Kataura plot

J. Jiang et al. *Phys. Rev.* B75 035405 and 035407(2007)





κ=2 is used for E22(S) and E11(M)

$$E^{\log} = 0.55(2p/3d_t)\log[3/(2p/3d_t)].$$

Justification of ETB+MB

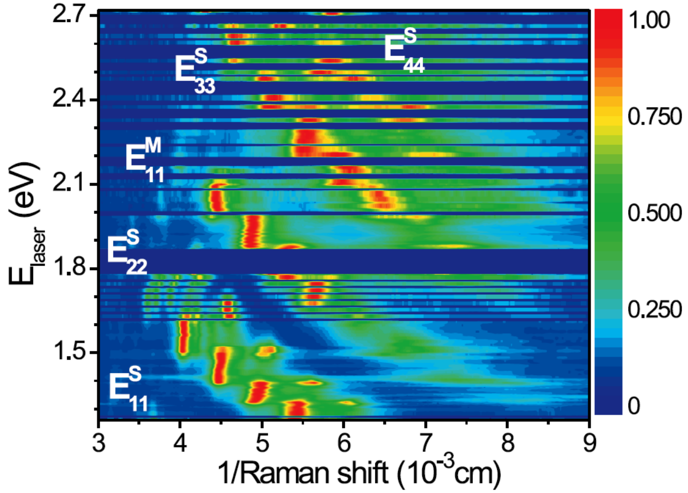
A. Jorio et al. Phys. Rev. (2006)

The origin of the large family spread in Kataura plot - single particle part

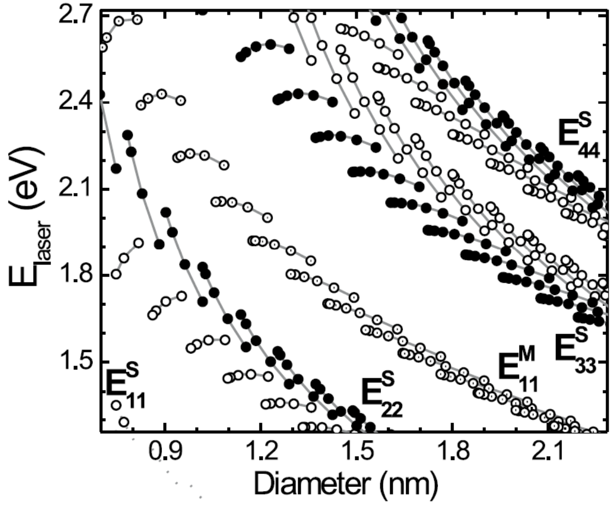
E33/E44 problem: exciton? exciton!

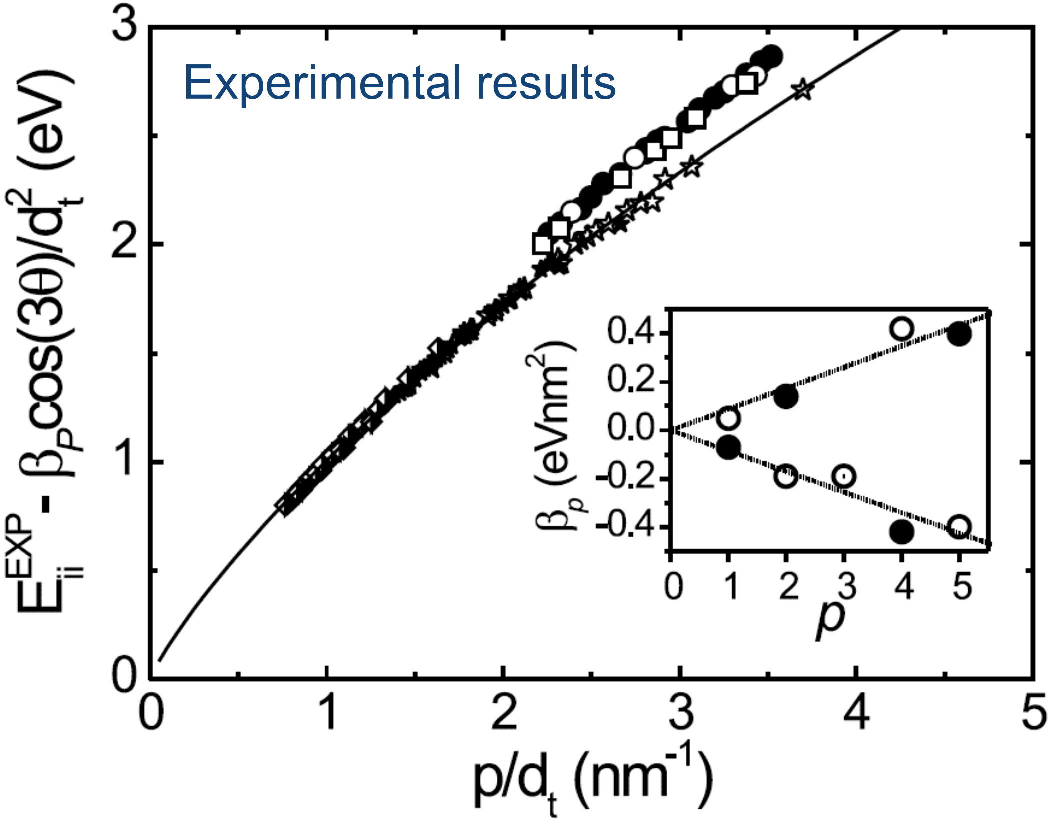
P. T. Araujo et al., Phys. Rev. Lett. 98, 067401 (2007)
T. Michel, et al. Phys. Rev. B75, 155432 (2007)

experiment



calculation



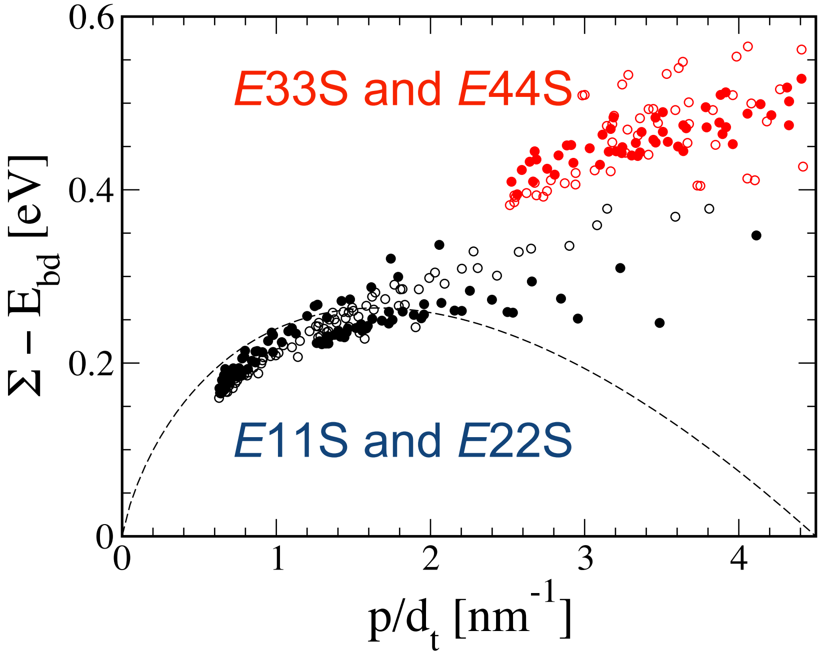


E_{33}^S and *E_{44}^S* do not follow a logarithmic correction

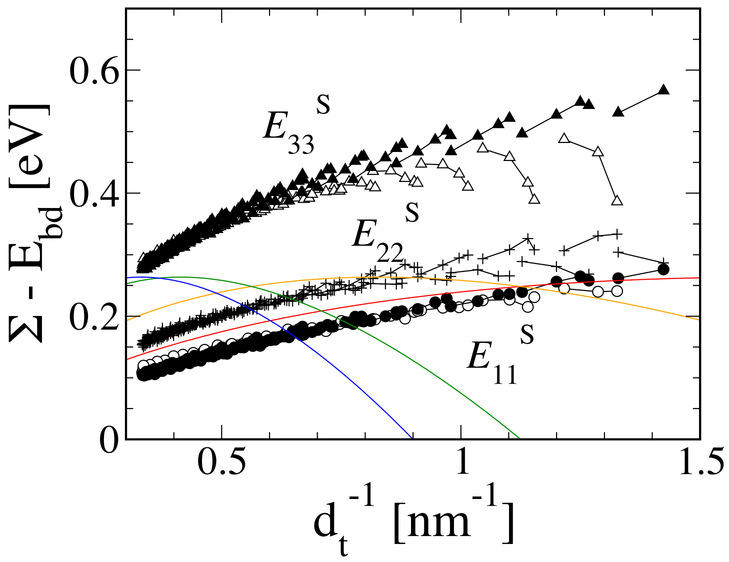
Chirality dep. of many body effects for E33 and E44

K. Sato et al., in press, Vib. Spec. (2007)

Exciton energy (Ω) = Single particle energy (ε) + Many body energy ($\Sigma - E_{\mathrm{bd}}$)



$$E^{\log} = 0.55(2p/3d_t)\log\left[3/(2p/3d_t)\right]$$



p = 1 (red), 2 (orange), 4 (green), 5 (blue)

○: Type I,
●: Type II

Large spread in family pattern

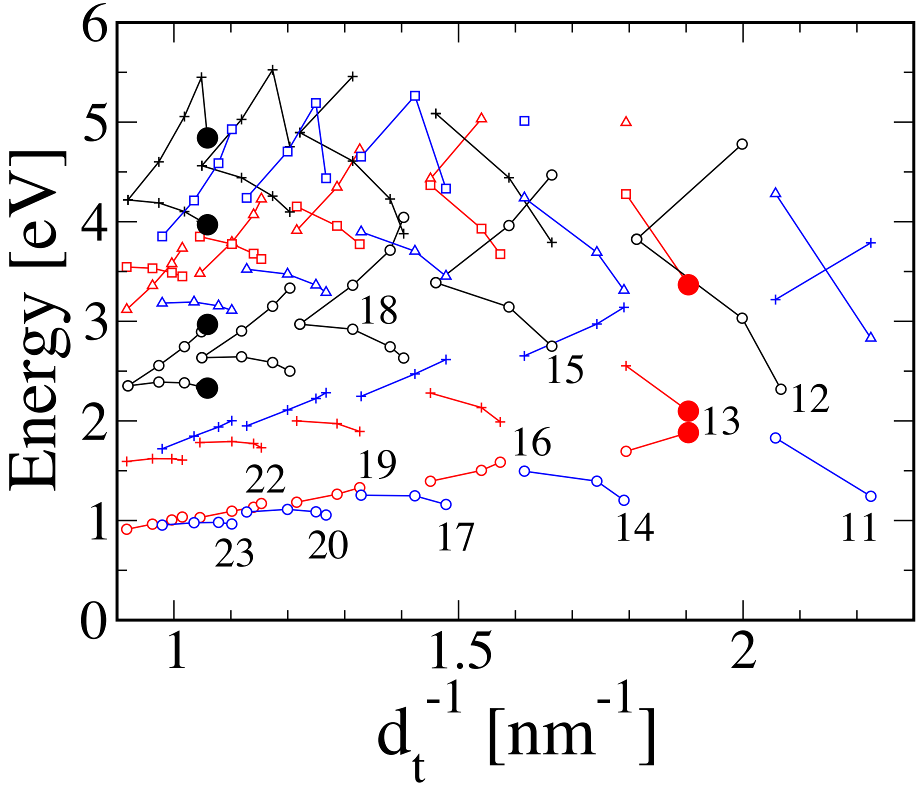
E_{11}^{S} and E_{22}^{S} (Black) : single particle energy (SPE)

E_{33}^{S} and E_{44}^{S} (Red): SPE + many body energy

Exciton Kataura plot: small diameter region
— What is this discontinuity? —

K. Sato et al., Phys. Rev. B in press, (2007)

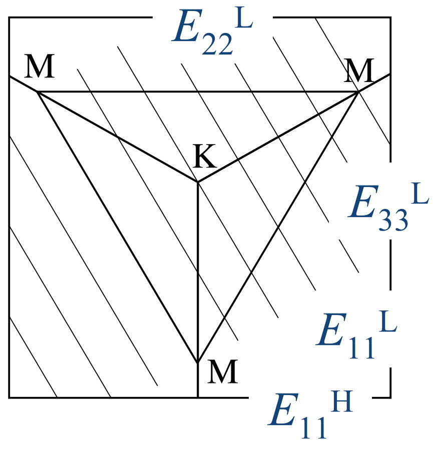
A_2 exciton, spin singlet, κ = 2.22

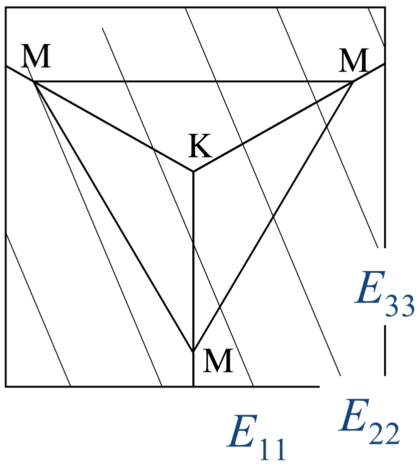


the number of E_{ii} in the triangle

$$n \neq m \quad n < 2\mu < 2n + m$$

$$n = m \quad n + m < 4\mu < 3(n + m)$$





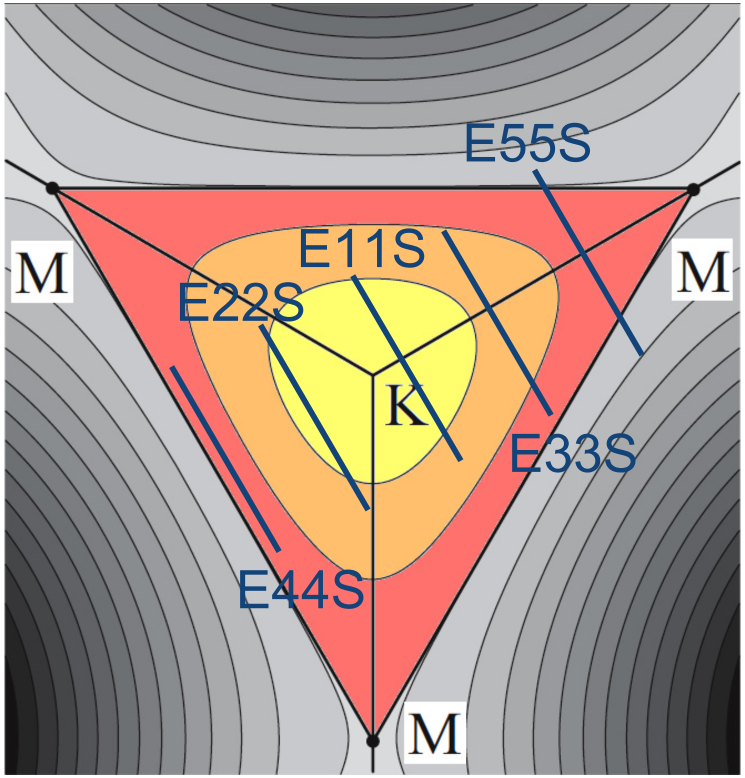
(12,0) Metal

E_{ii} is up to E_{33}^L

(6,1) Type I

E_{ii} is up to E_{33}

Trigonal warping and many body effects change the order of Eii



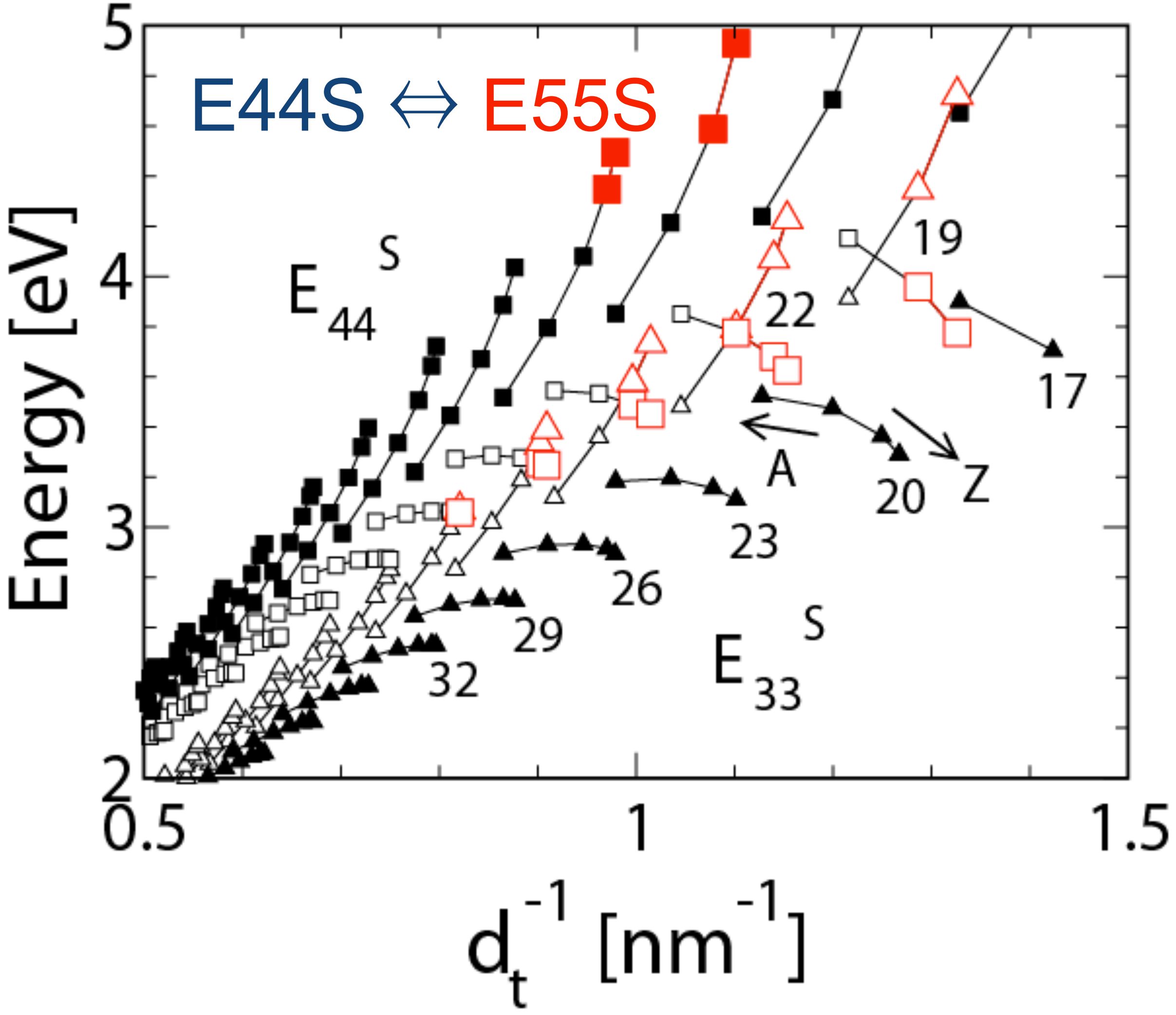
E55S < E44S

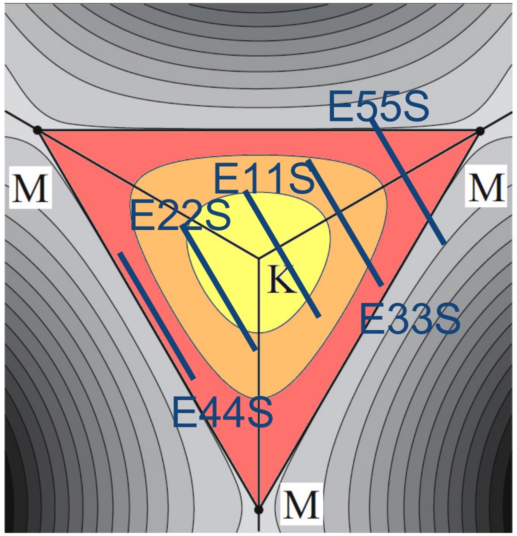
k_{ii} position is not always continuous for (2n+m) family

→ G’–band Raman

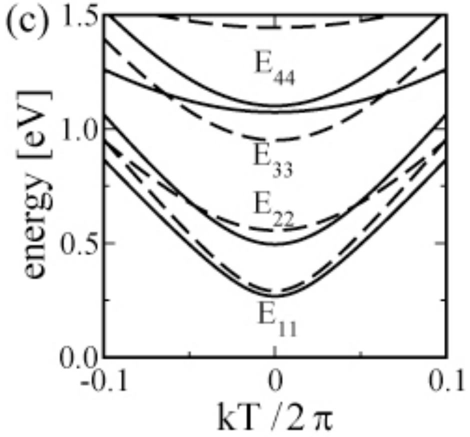
E33S, E44S exciton Kataura’s Plot

Crossing occurs:
E33S ⇔ E44S

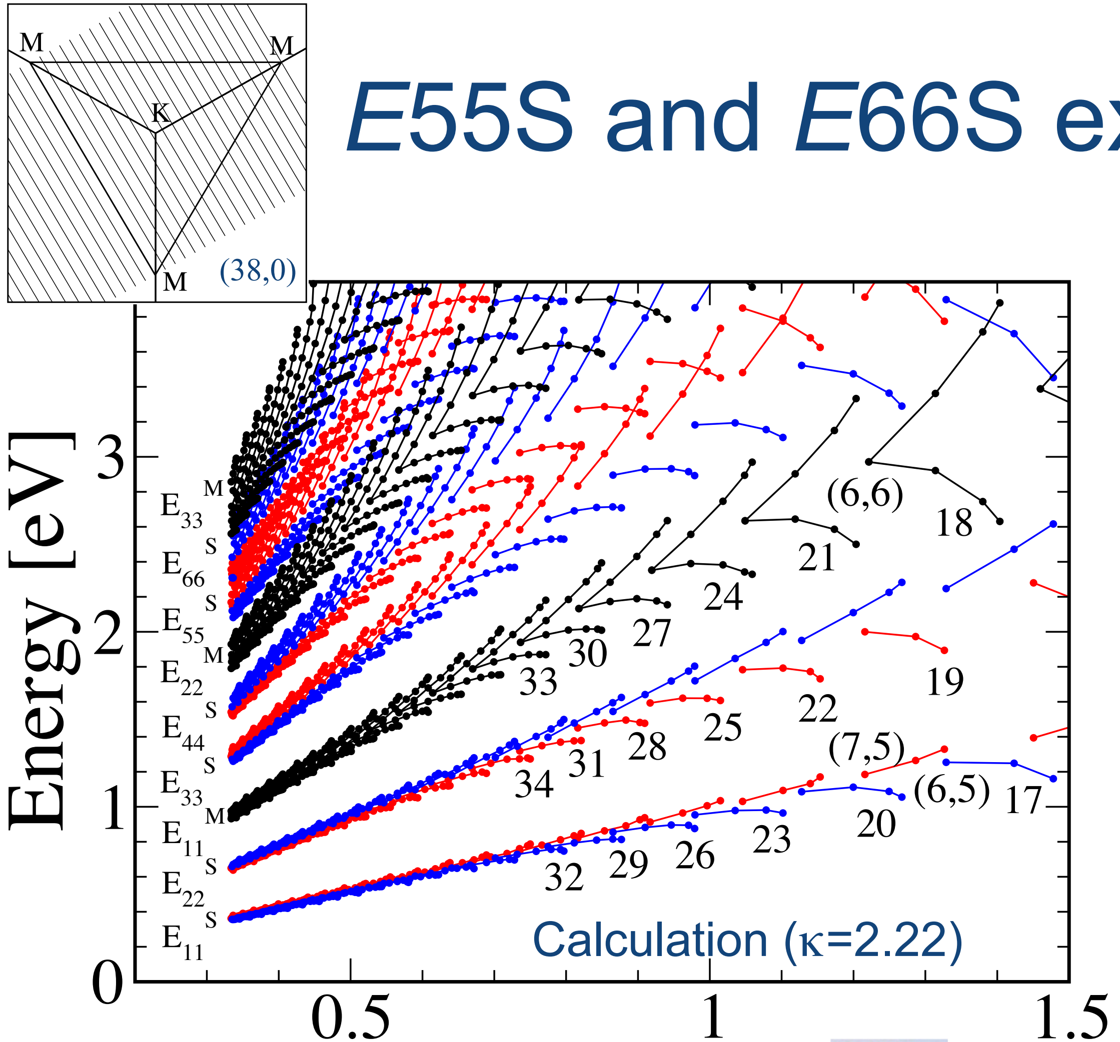




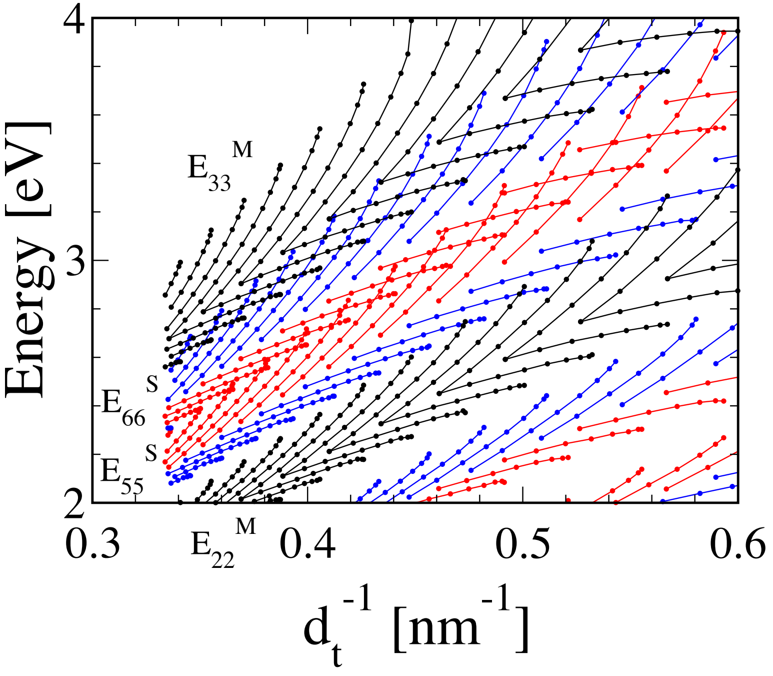
definition of Eii

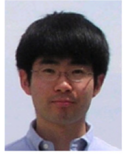


*E*55S and *E*66S exciton Kataura plot



A$_2$ exciton, spin singlet,
κ = 2.22



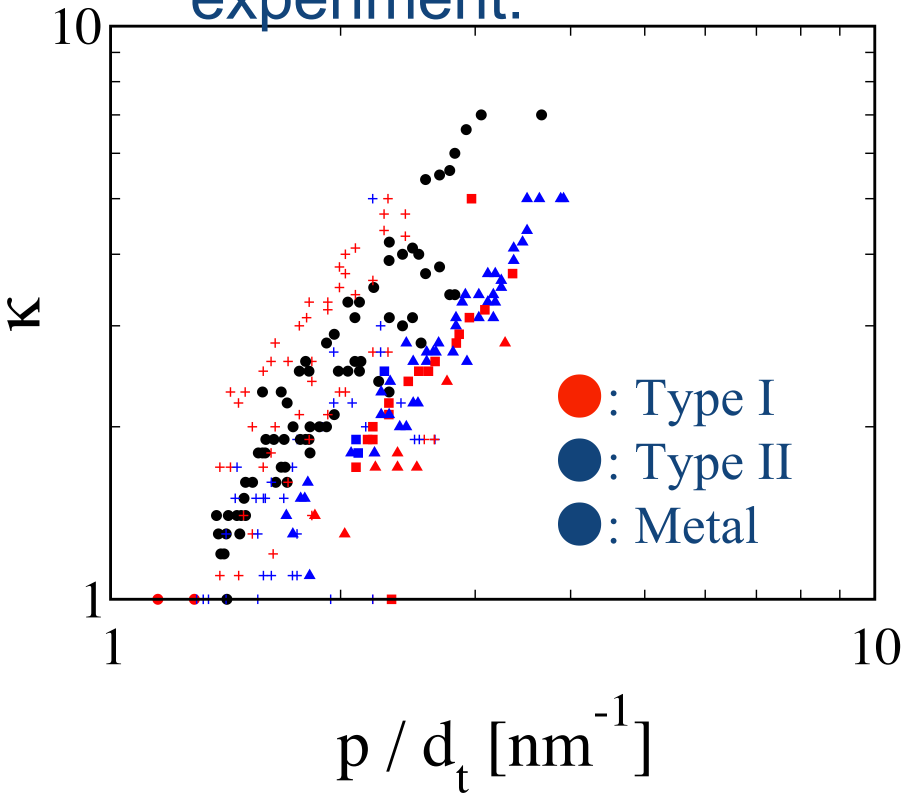


●: Type I
●: Type II
●: Metal

A large overlap of E55S and E66S for type I
⇒ trigonal warping effect

Diameter dependence of κ

Adjust κ in calculation to reproduce experiment.

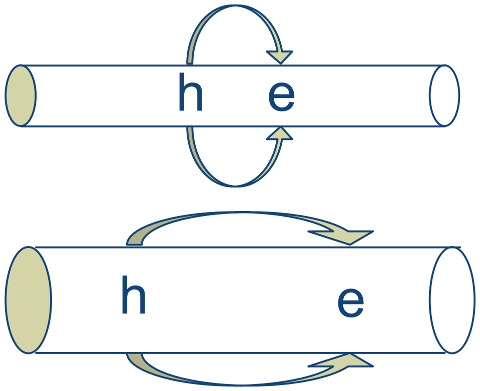


Symbols: E_{11} (○), E_{22} (+), E_{33} (△), E_{44} (□),
p = 1, 2, 3, … (E_{11}^{S}, E_{22}^{S}, E_{11}^{M}, …)

$$\kappa \propto p/d_t^{-1.24}$$

for two samples
- Maruyama
- Hata

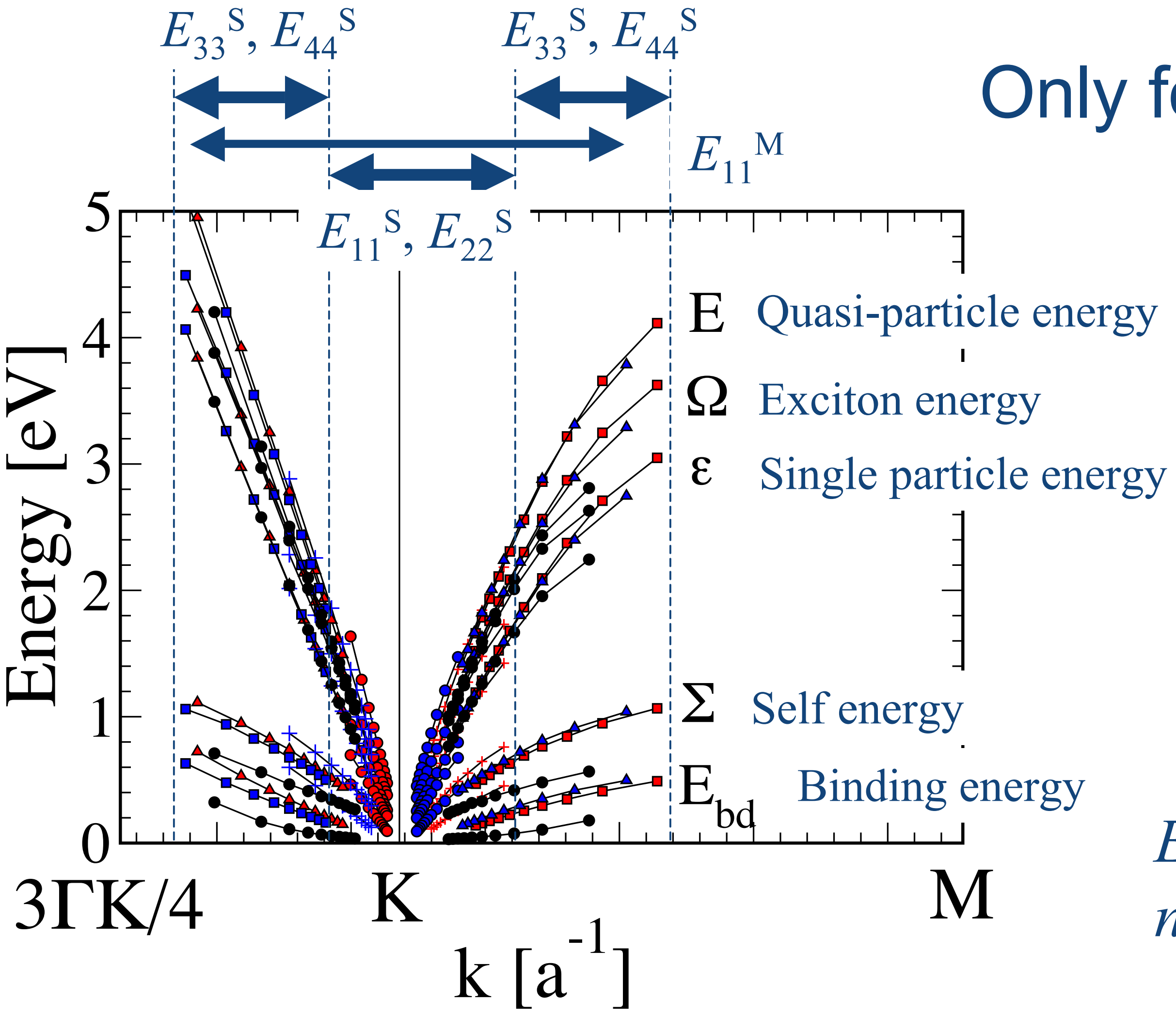
Environmental effect



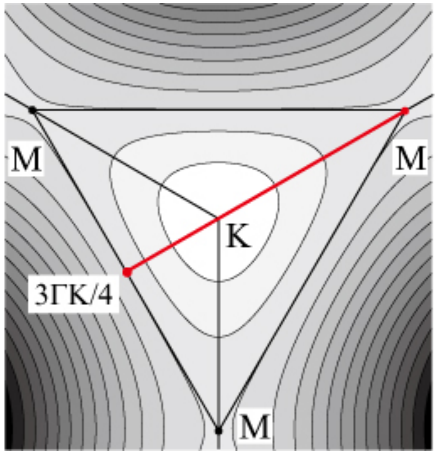
Energies as a function of wave vector

K. Sato et al., *Phys. Rev.* **B** *in press* (2007)

Only for zigzag NTs



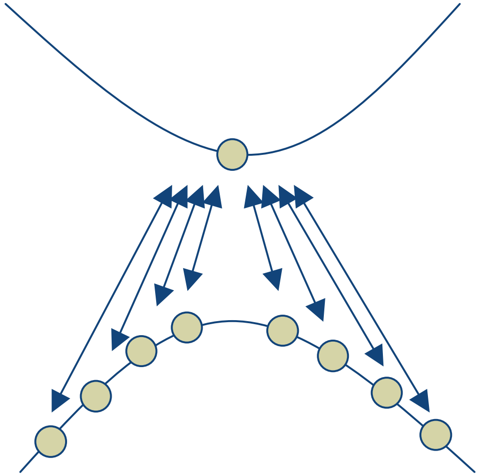
●: Type I, ●: Type II, ●: Metal



E_{ii} is up to E_{44}^{S} and E_{22}^{M}

$n = 9, 10, \ldots, 38$

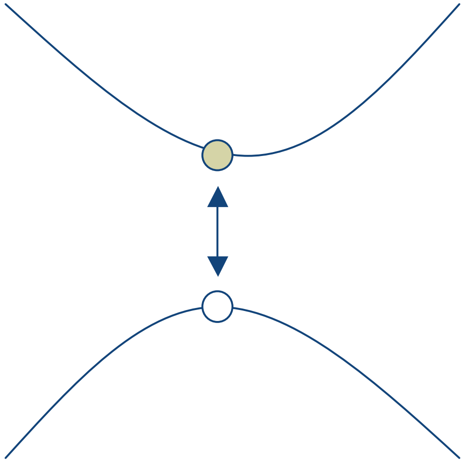
Why is self energy larger than E_{bd}?



self energy

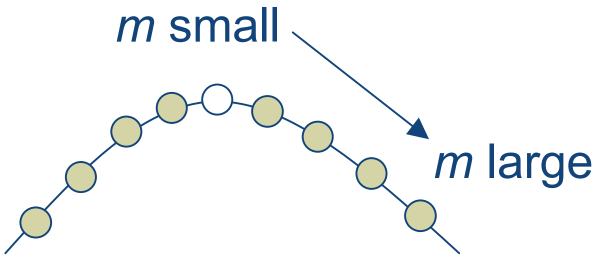
Reduced mass

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

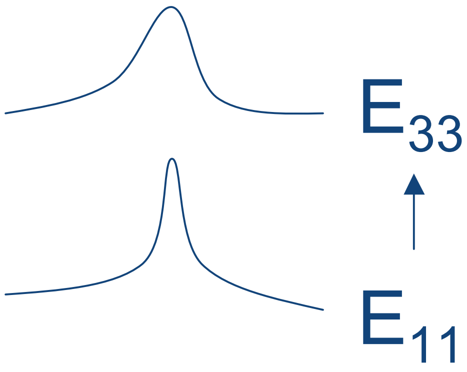


E_{bd}

effective mass



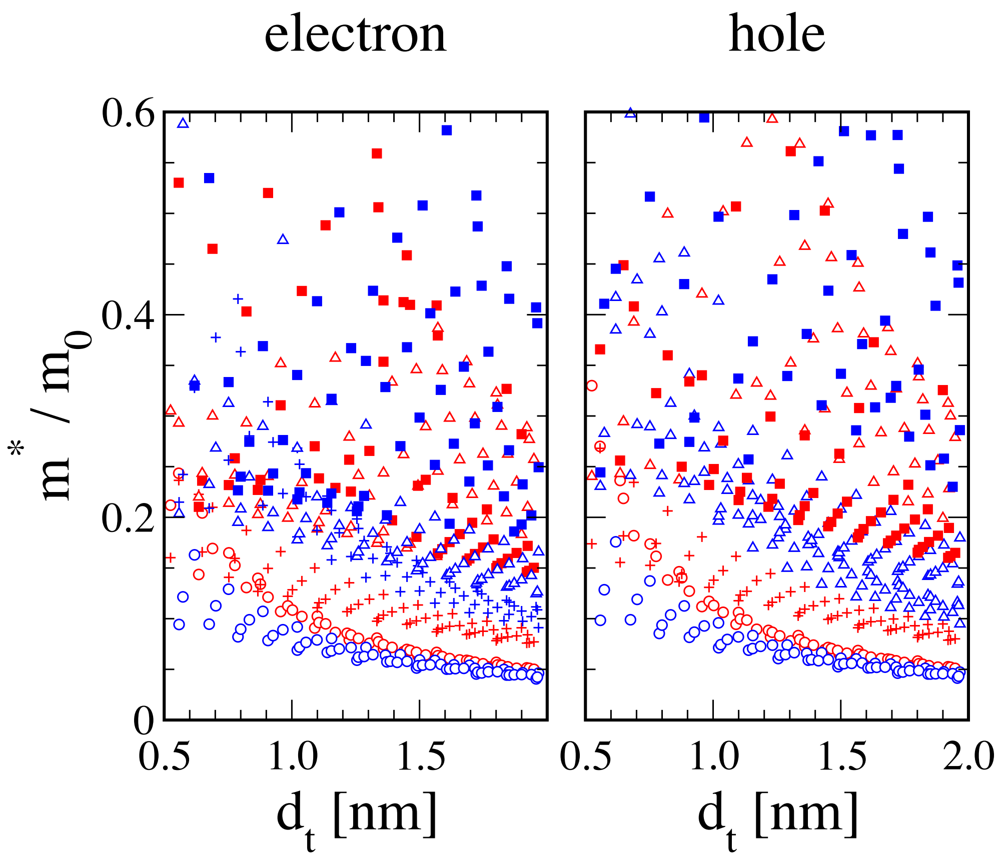
Z_k delocalization in k



$$\mu_{\text{SELF ENERGY}} > \mu_{\text{BINDING ENERGY}}$$

ETB Effective mass

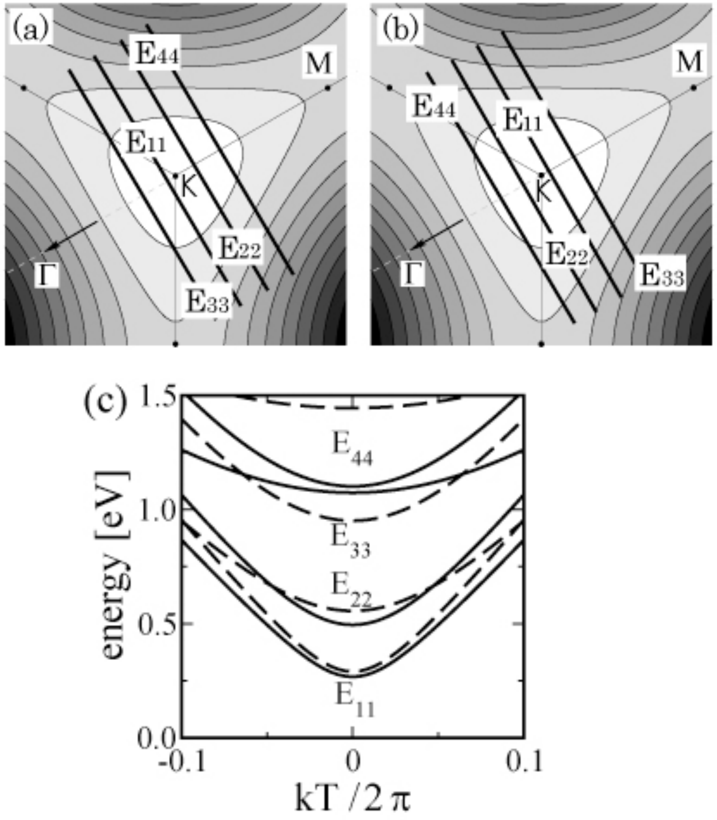
K. Sato et al. *Phys. Rev.* **B** *in press* (2007)



●: Type I

●: Type II

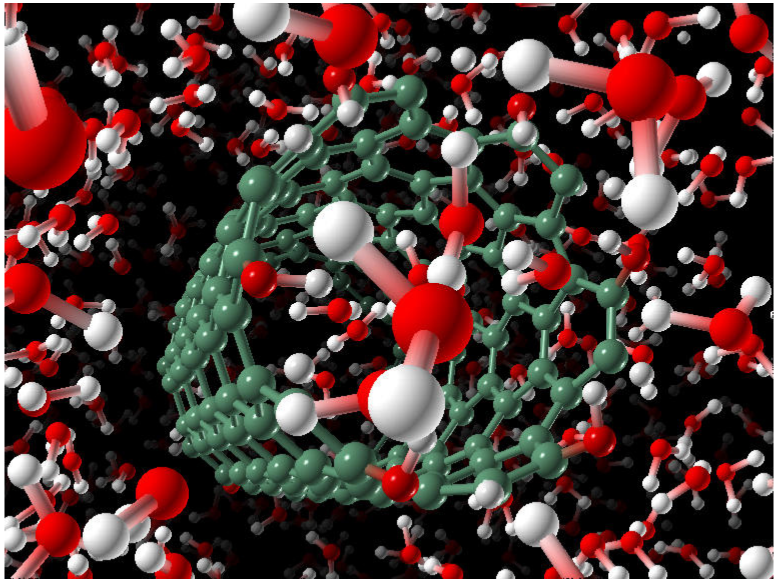
m_0 : electron mass

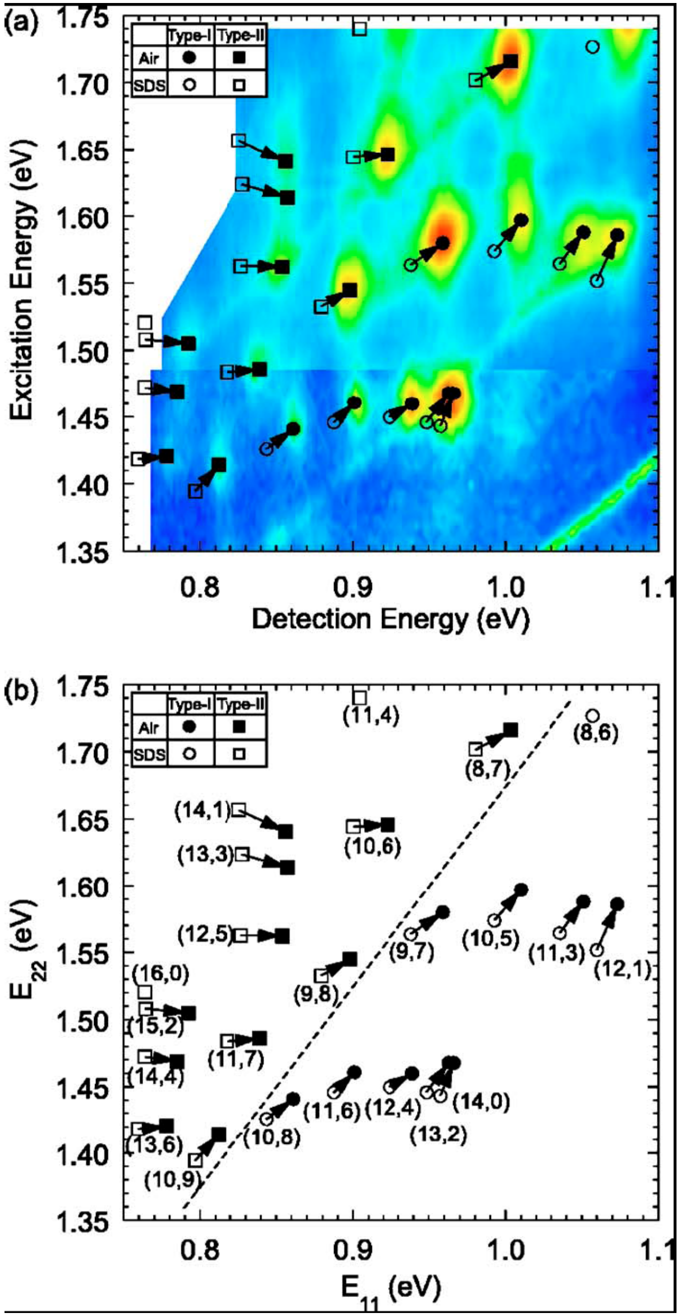


$$\frac{1}{m} \propto \frac{\partial^2 E}{\partial k^2}$$

Environmental Effect of SWNTs

ΔEii (0-80meV) by surronding materials





Dielectric screening of many body effect.

Chirality dependent, type dependent

Effective mass

Y. Ohno et al., Phys. Rev. B **73**, 235427 (2006)

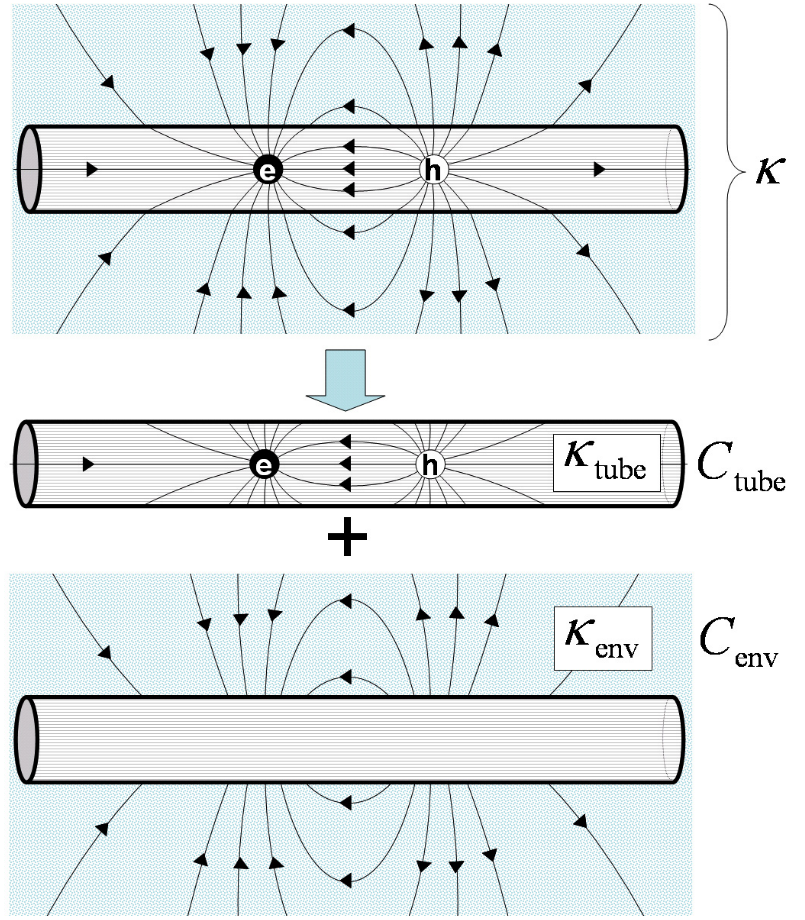
Environmental Effect of SWNTs

Bethe-Salpeter equation with tight-binding wavefunction

$$\left\{[E(\boldsymbol{k}_\mathrm{c})-E(\boldsymbol{k}_\mathrm{v})]\delta(\boldsymbol{k}_\mathrm{c}',\boldsymbol{k}_\mathrm{c})\delta(\boldsymbol{k}_\mathrm{v}',\boldsymbol{k}_\mathrm{v})\right.$$

$$\left.+K(\boldsymbol{k}_\mathrm{c}'\boldsymbol{k}_\mathrm{v}',\boldsymbol{k}_\mathrm{c}\boldsymbol{k}_\mathrm{v})\right\}\Psi^n(\boldsymbol{k}_\mathrm{c}\boldsymbol{k}_\mathrm{v})=\Omega_n\Psi^n(\boldsymbol{k}_\mathrm{c}'\boldsymbol{k}_\mathrm{v}')$$

$$|\Psi_{\boldsymbol{q}}^n>=\sum_{\boldsymbol{k}} Z^n_{\boldsymbol{k}\mathrm{c},(\boldsymbol{k}-\boldsymbol{q})\mathrm{v}}c^{\dagger}_{\boldsymbol{k}\mathrm{c}}c_{(\boldsymbol{k}-\boldsymbol{q})\mathrm{v}}|0>$$



Dielectric screening effect within the RPA

$$W=V/\kappa\epsilon(\boldsymbol{q})$$

$\epsilon(\boldsymbol{q})$ π electrons

κ core-electrons
& surrounding materials

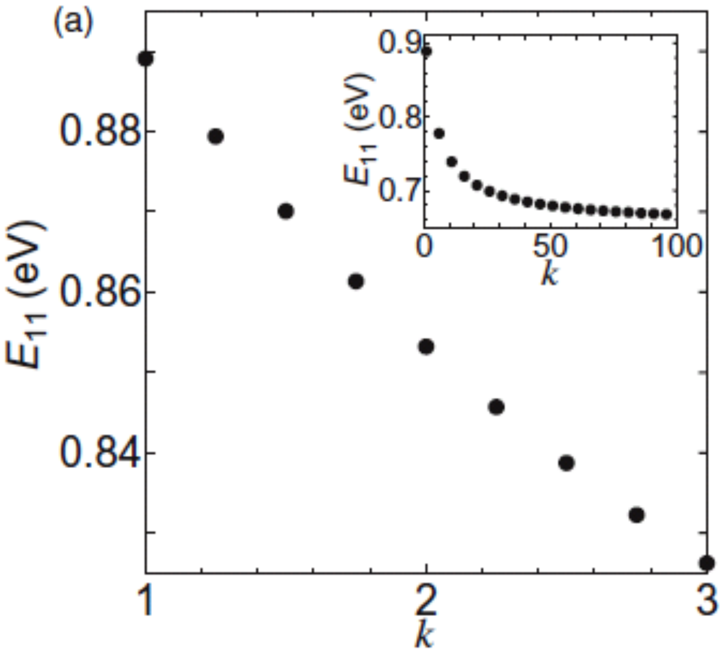
Connection of the dielectric constants

$$\frac{1}{\kappa}=\frac{C_{\mathrm{tube}}}{\kappa_{\mathrm{tube}}}+\frac{C_{\mathrm{env}}}{\kappa_{\mathrm{env}}}$$ (analogy to the serial connection of two capacitors)

Y. Miyauchi, R. Saito, K. Sato, Y. Ohno, S. Iwasaki, T. Mizutani, J. Jiang, S. Maruyama, Chem. Phys. Lett 442, 394 (2007)

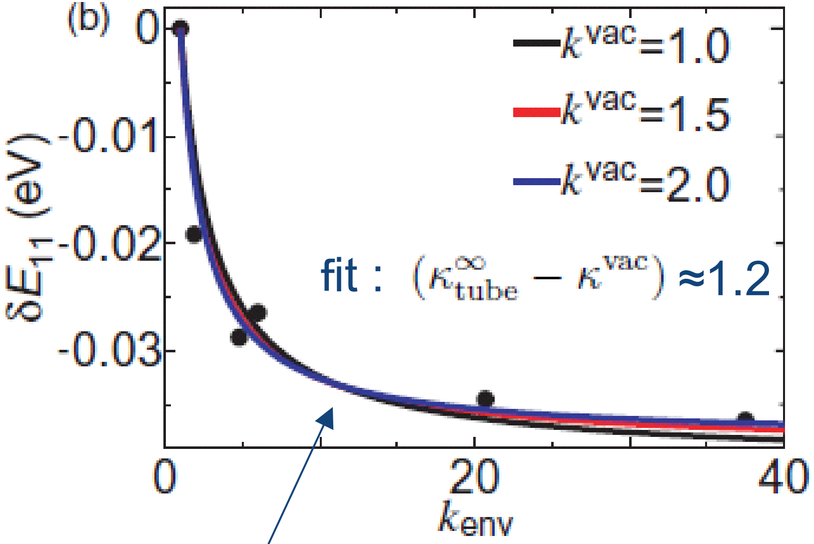
Exciton Transition Energy in Surrounding Dielectric Materials

Calculated E_{11} energy for a (9, 8) SWNT as a function of κ



- experiment

— theory



fit : $(\kappa_{\text{tube}}^{\infty} - \kappa^{\text{vac}}) \approx 1.2$

δE_{11} can be approximated as

$$\delta E_{11} = -A_{nm}(\kappa - \kappa^{\text{vac}})$$

$$\delta E_{11} = -A_{nm}(\kappa_{\text{tube}}^{\infty} - \kappa^{\text{vac}})\left(\frac{\kappa_{\text{env}} - 1}{\kappa_{\text{env}} + (\kappa_{\text{tube}}^{\infty} - \kappa^{\text{vac}})/\kappa^{\text{vac}}}\right)$$

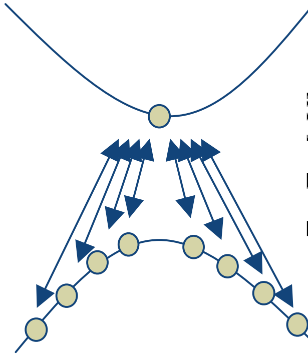
C_{tube}, C_{env} can be expressed using $(\kappa_{\text{tube}}^{\infty} - \kappa^{\text{vac}})$

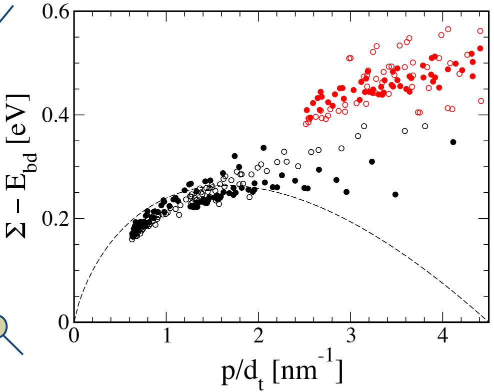
$$\frac{1}{\kappa} = \frac{C_{\text{tube}}}{\kappa_{\text{tube}}} + \frac{C_{\text{env}}}{\kappa_{\text{env}}}$$

κ when the dielectric constant of the environment is infinity

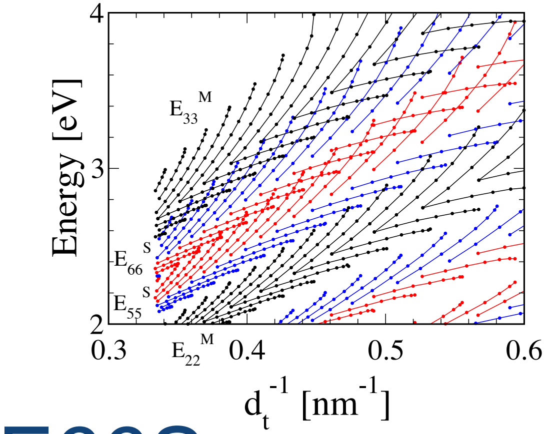
κ when the SWNT is placed in the vacuum

Y. Miyauchi, R. Saito, K. Sato, Y. Ohno, S. Iwasaki, T. Mizutani, J. Jiang, S. Maruyama, Chem. Phys. Lett 442, 394 (2007)

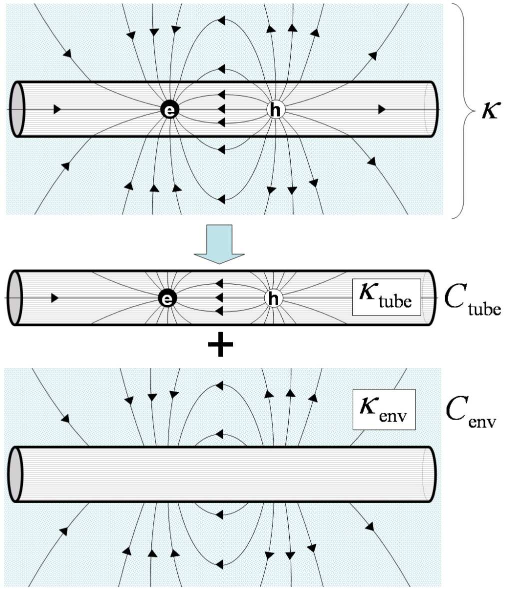


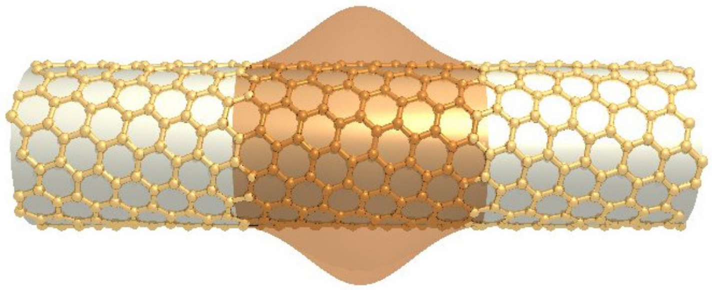


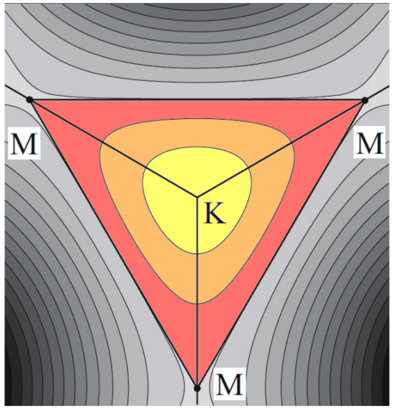
Summary



- Exciton Kataura-plot up to E33M, E66S
  - Chirality dep. of E33(E44) many body effect
  - Environmental effect can be modeled
  - Discontinuity of Eii for type I, crossing
    - Important for checking the calculation
    - G' band, environmental effect







What is “Shiran”?

“ShiRan” is impolite expression “I do not know.” ?

霊芝/レイシ/Reishi/Ganogerma lucidum

サルノコシカケ科マンネンタケ

蘭草/ランソウ/Ransou/Eupatorium fortunei

キク科フジバカマ属

Originated from a famous Chinese philosopher

Confucius (c. 551-479 BCE)「孔子家語」一節

Kyoto University President, Prof. Kinoshita put this name for his wishing to produce precious medical doctors like these rare medical plants.