Metal-Semiconductor Transitions in Armchair Carbon Nanotubes by Symmetry Breaking

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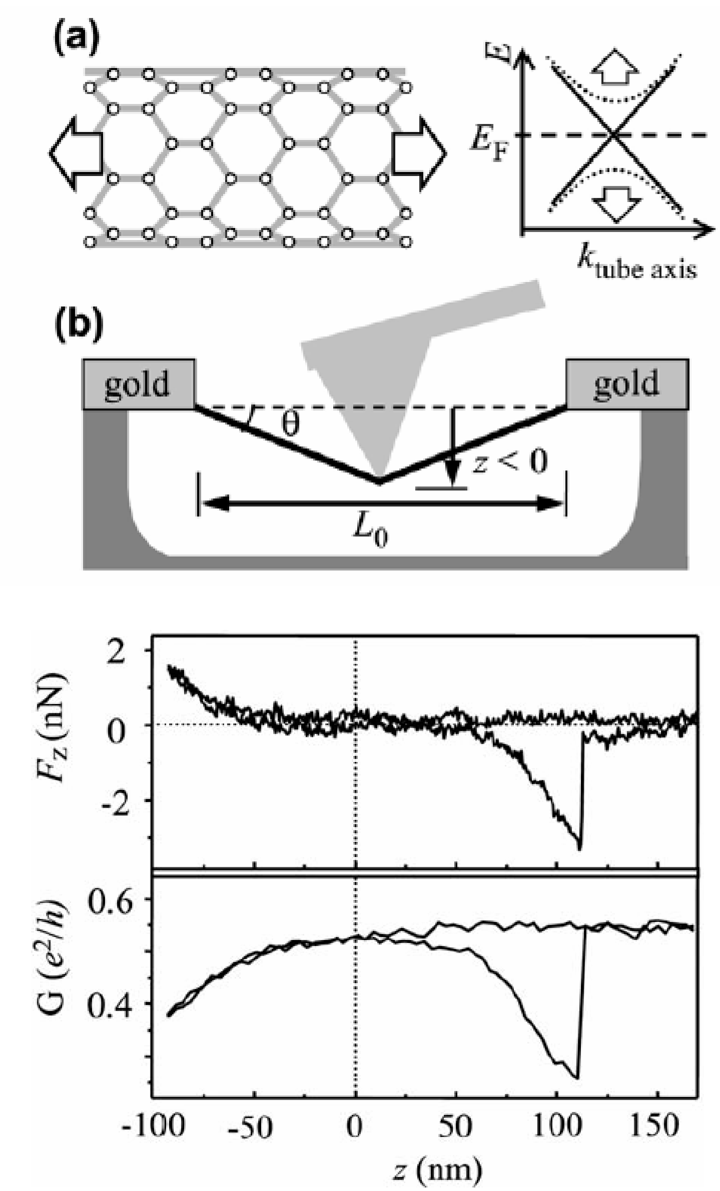
Metal-Semiconductor Transition and *Semiconductor-Metal Transition* in carbon nanotubes (general)

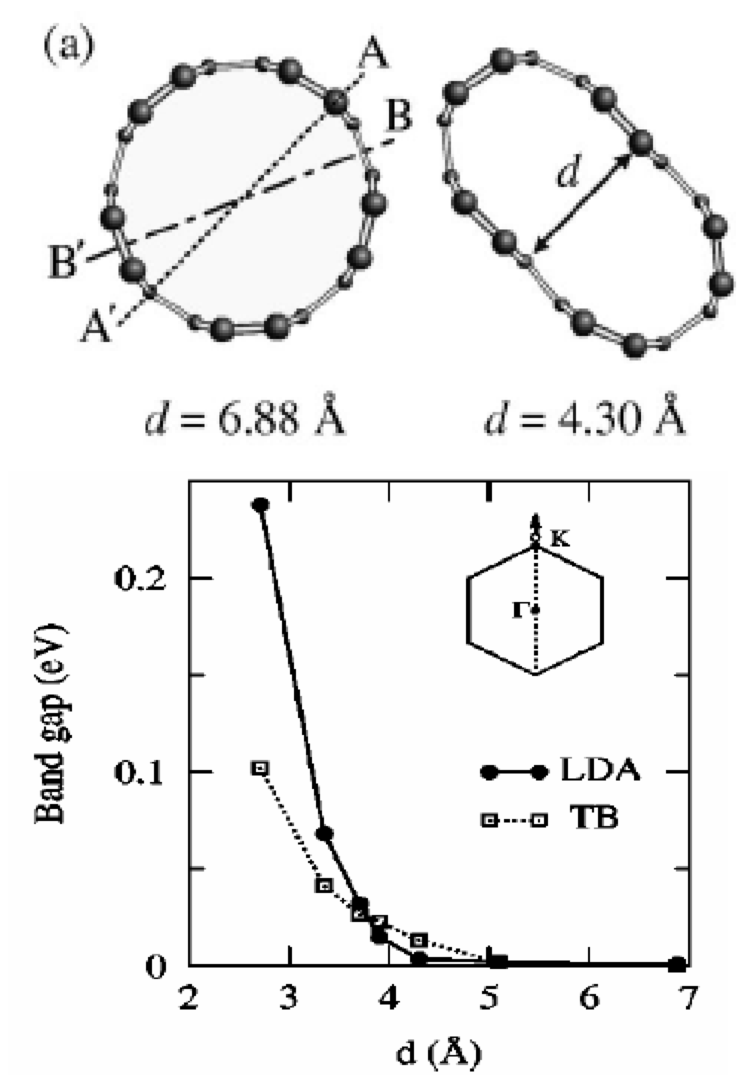
- Mechanical deformation
  - Stretching , bending, squashing, twisting, defects, etc
- Electro-magnetic modulation
  - Electric field, magnetic field, etc
- Chemical, biological decoration, functionalization
- And more…

Stretching



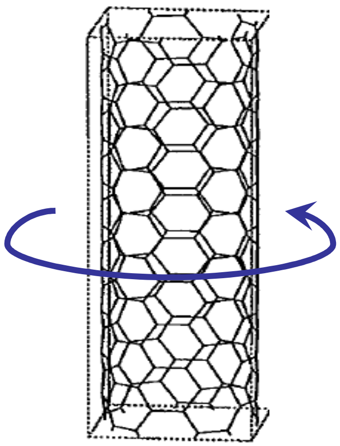
Minot et al, *PRL* **90**,156401 (2003)

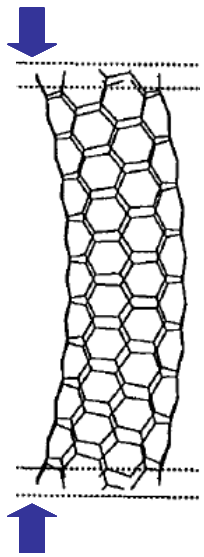
Squashing



K.J. Chang et al, *Phys.Rev.B* **60**, 10656(1999).

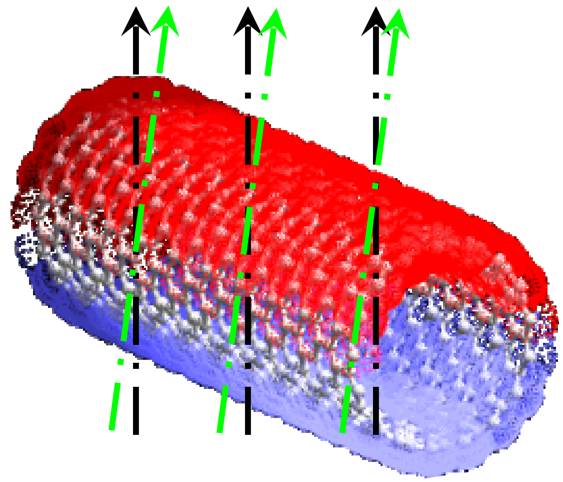
Twisting **Bending**

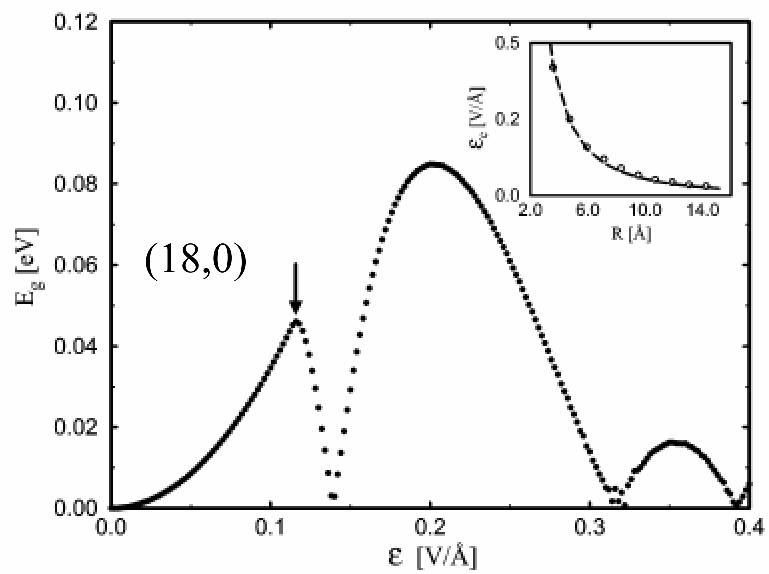




Kane and Mele, *PRL* **78**, 1932 ,(1997)

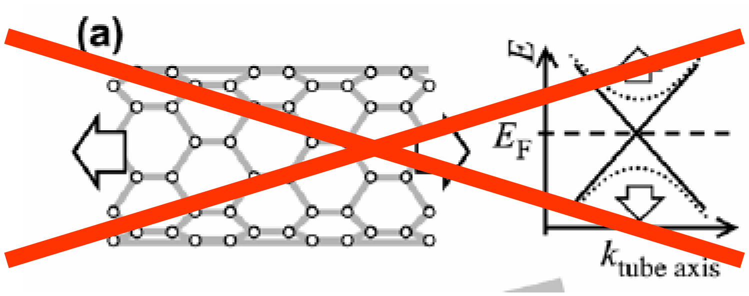
Uniform electric field

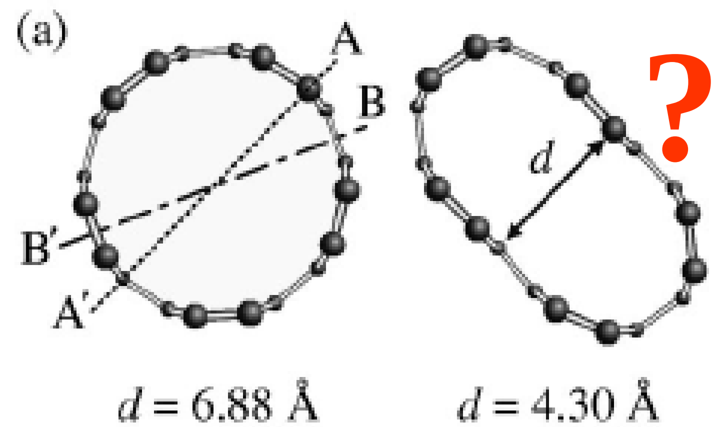


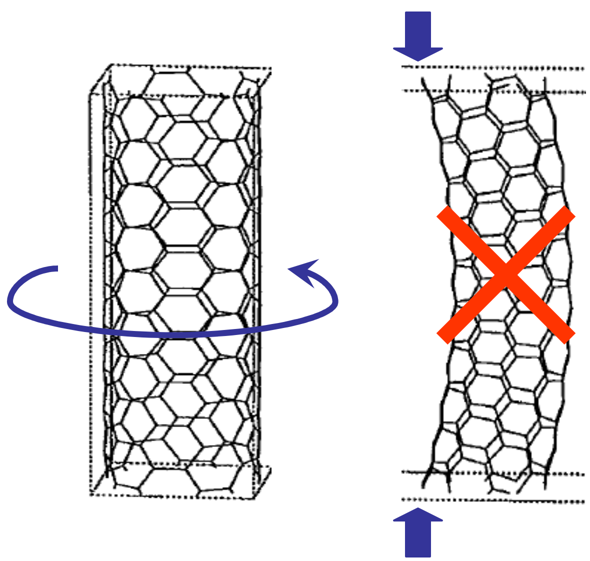


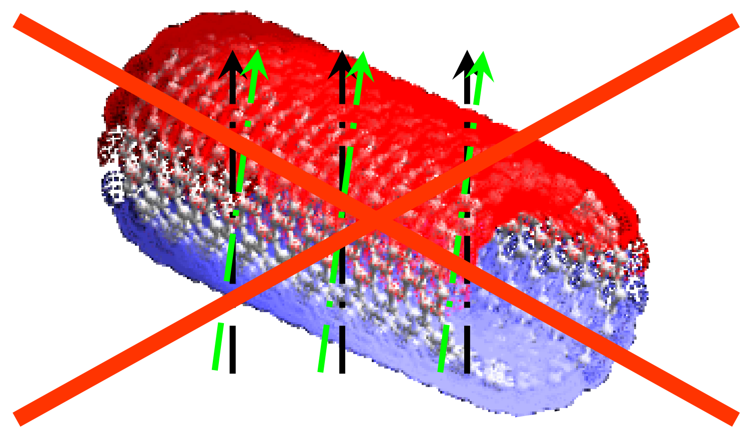
Li, Rotkin, ,Ravaioli, *Nano Letter* 3, 183 (2003)

Not all means induce a band gap in armchair CNTS!



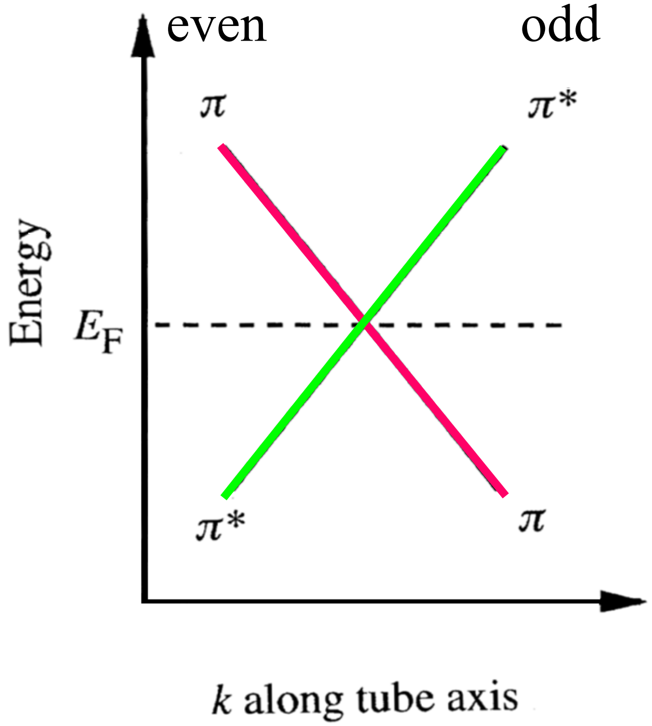


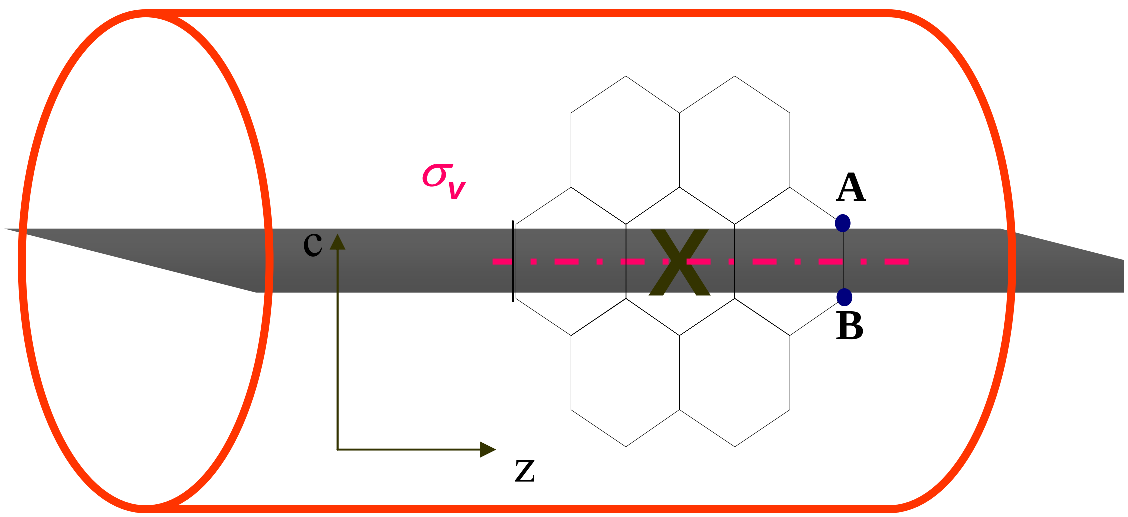




Mirror symmetry of armchair CNTs

Parities about σ_v





Outline

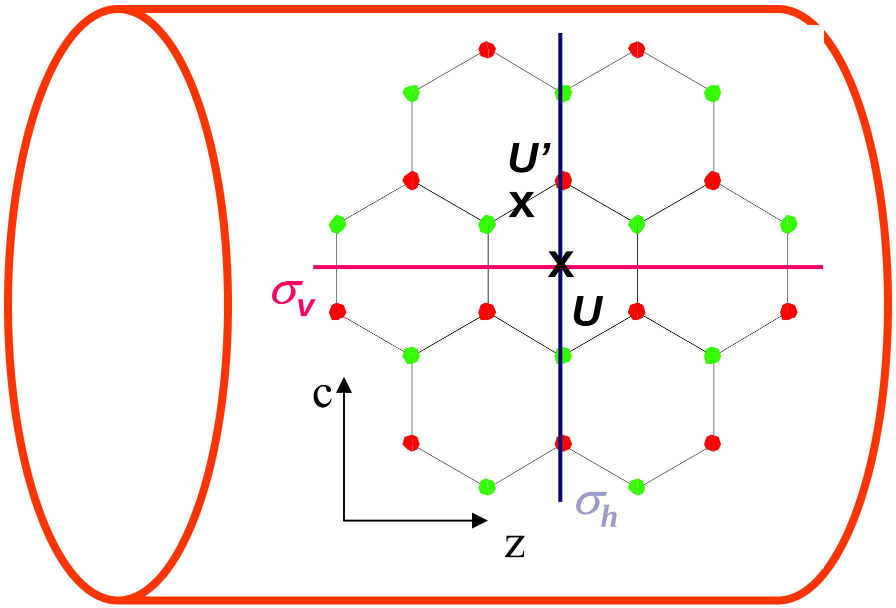
- Apply circumferential electrostatic potential

$$V_q(\theta) = V_{q0}\cos(q\theta)$$
$$V(\theta) = \sum_q V_q$$

- Selection rules of M-S transition
  - Symmetry of external perturbation
  - Angular quantum number q
  - Index n of (n,n) armchair CNT

- Method
  - Tight-Binding calculation
  - Degenerate perturbation theory

Symmetry of Armchair CNTs



	$\|\pi\rangle$	$\|\pi^*\rangle$
m	n	n
σ_v	+1	-1
σ_h	+1	+1
U	-1	+1
U'	-1	+1

Conservation law of parities

$$\mathrm{P}(|i\rangle) * \mathrm{P}(V_q) * \mathrm{P}(|f\rangle) = 1$$

When **P(V) = 1**, $|i\rangle \Leftrightarrow |f\rangle$ are forbidden if they possess opposite parities.

Rule 1

All symmetries about

(1) vertical mirror planes σ_{vi}
(2) C_2 rotation axes U ,U'

must be broken simultaneously.

Angular quantum number *m*

Angular quantization

$$k_x = m\frac{1}{2\pi R}, m = 1,2,\ldots 2n$$

$$V_q = V_0 \sin(q\theta)$$

Conservation law of *m*

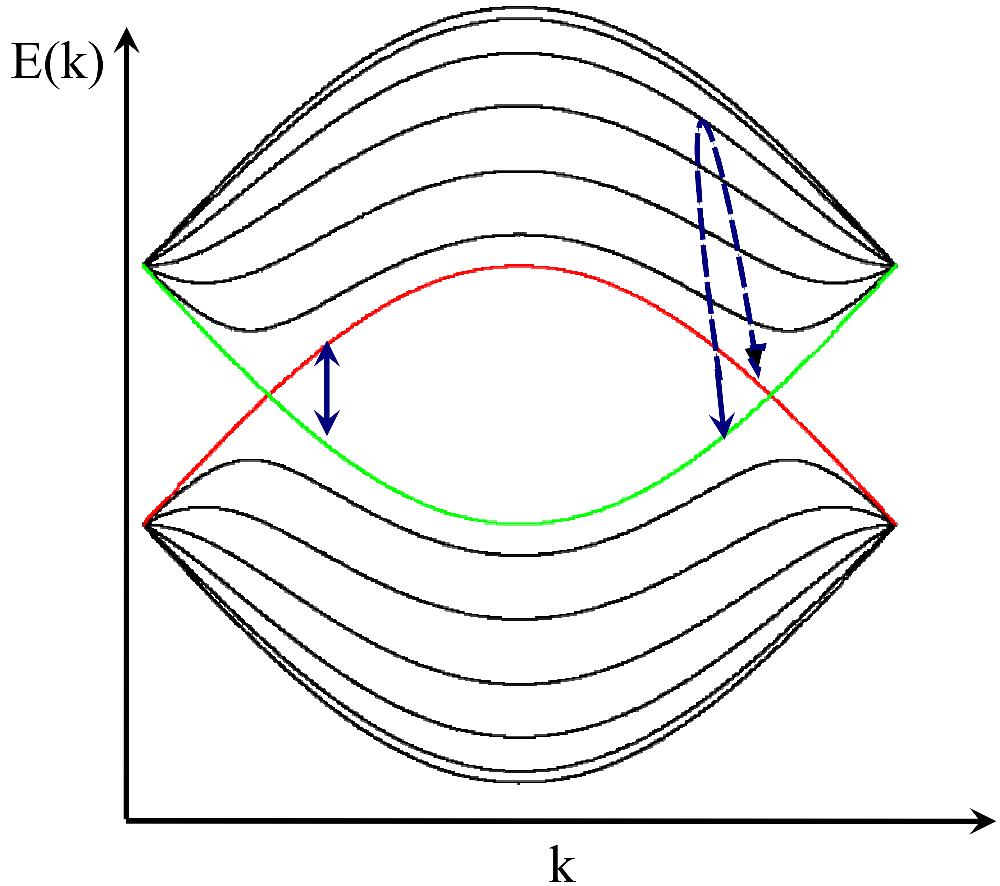
$$m_i + q = m_f$$

Coupling order

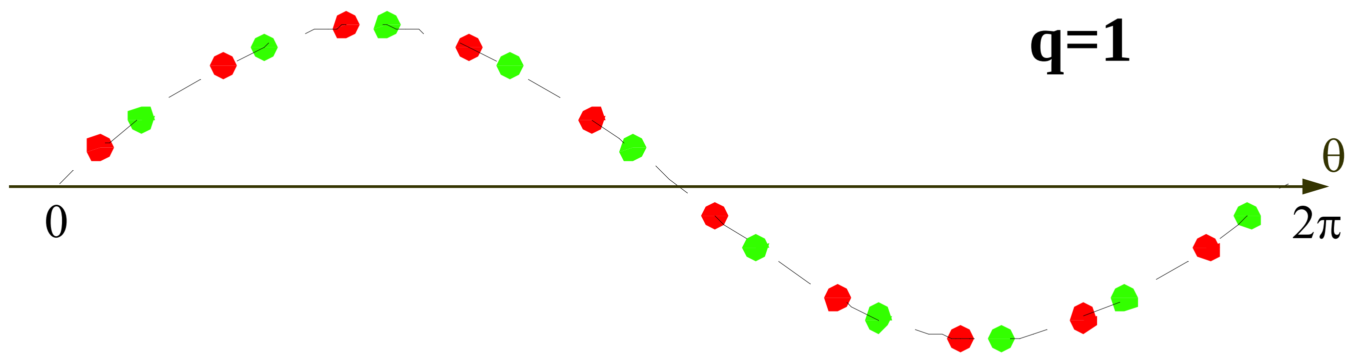
$$\mu = \mu(q)$$

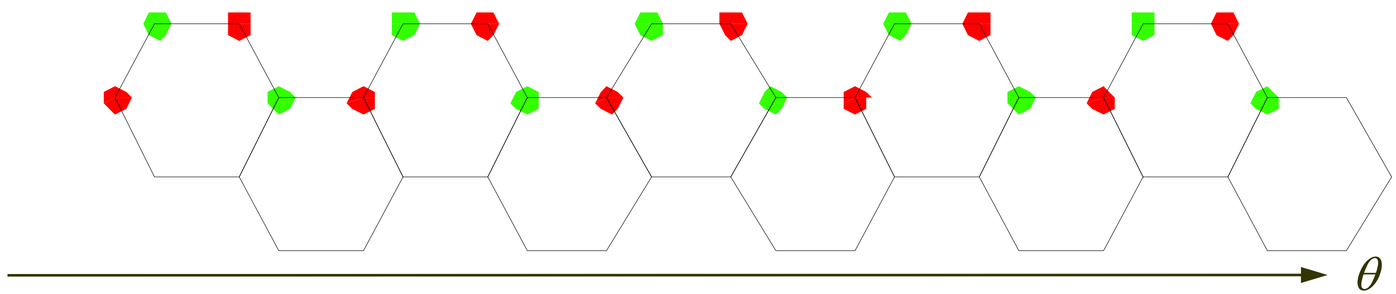
$$E_g \propto V_0^{\mu}$$

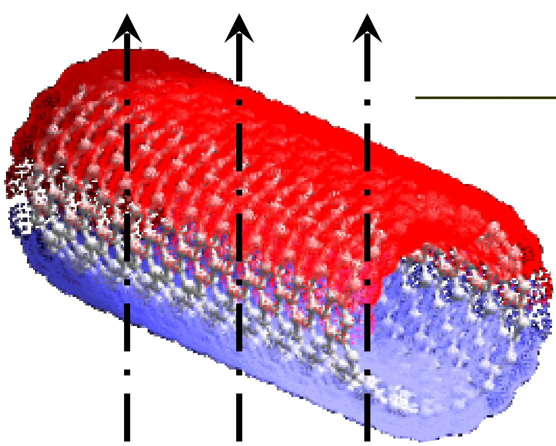
Band structure of (6,6) CNT

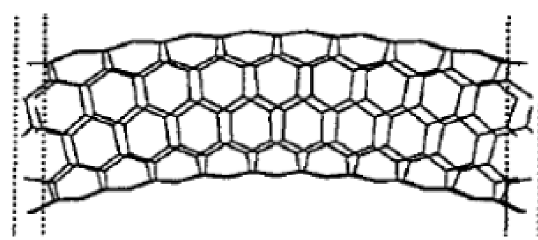


Angular quantum number of potential

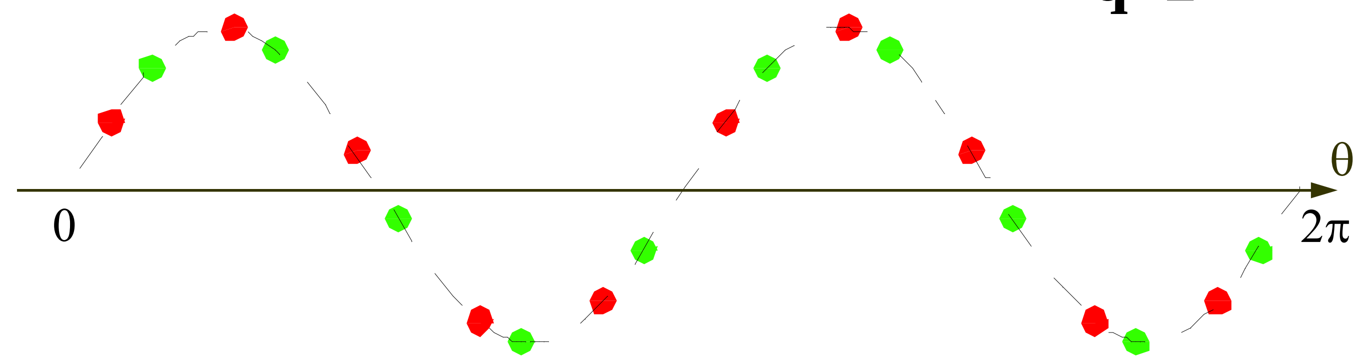


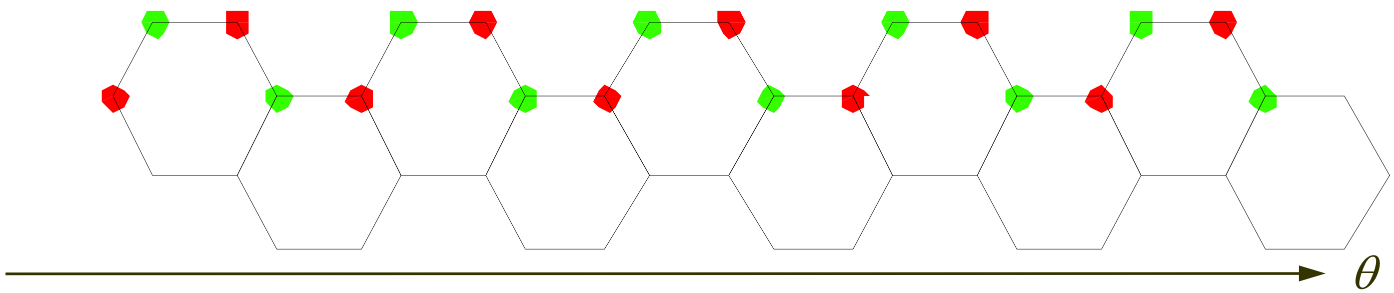


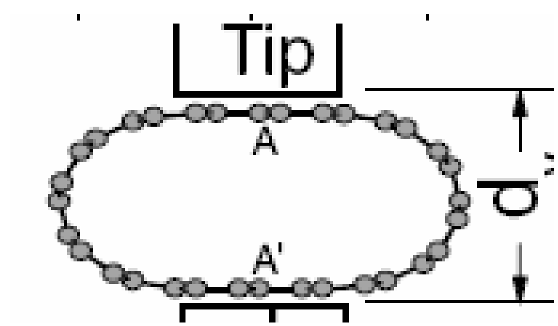




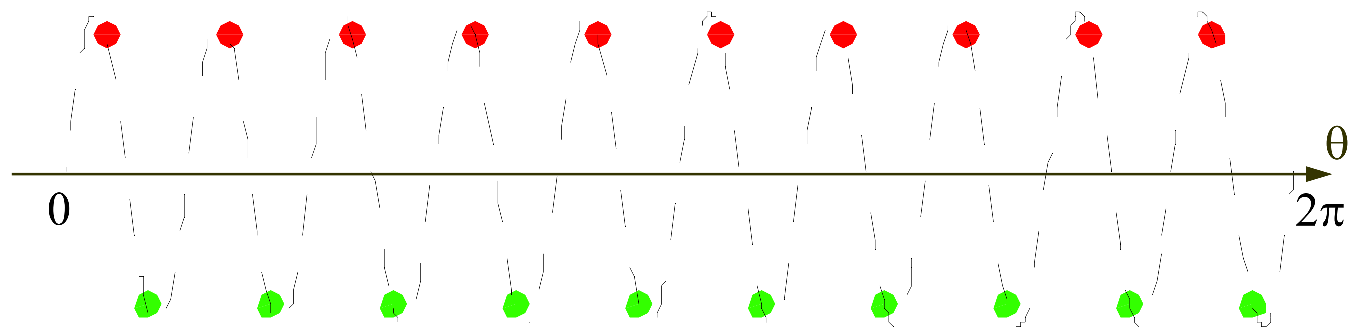
q=2

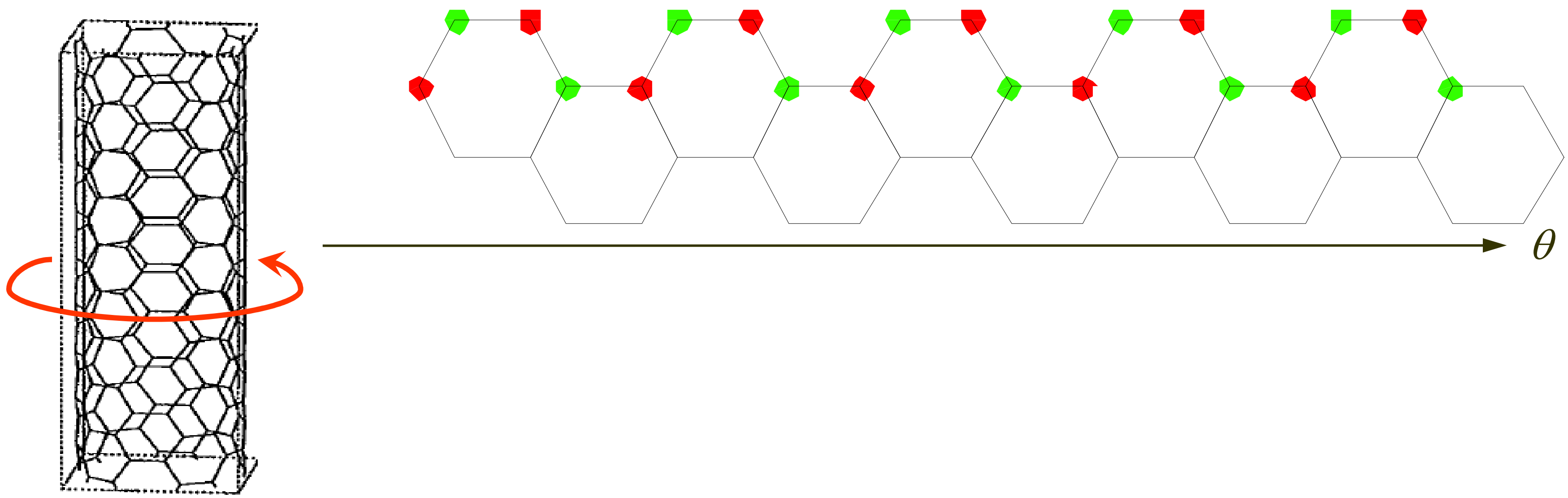




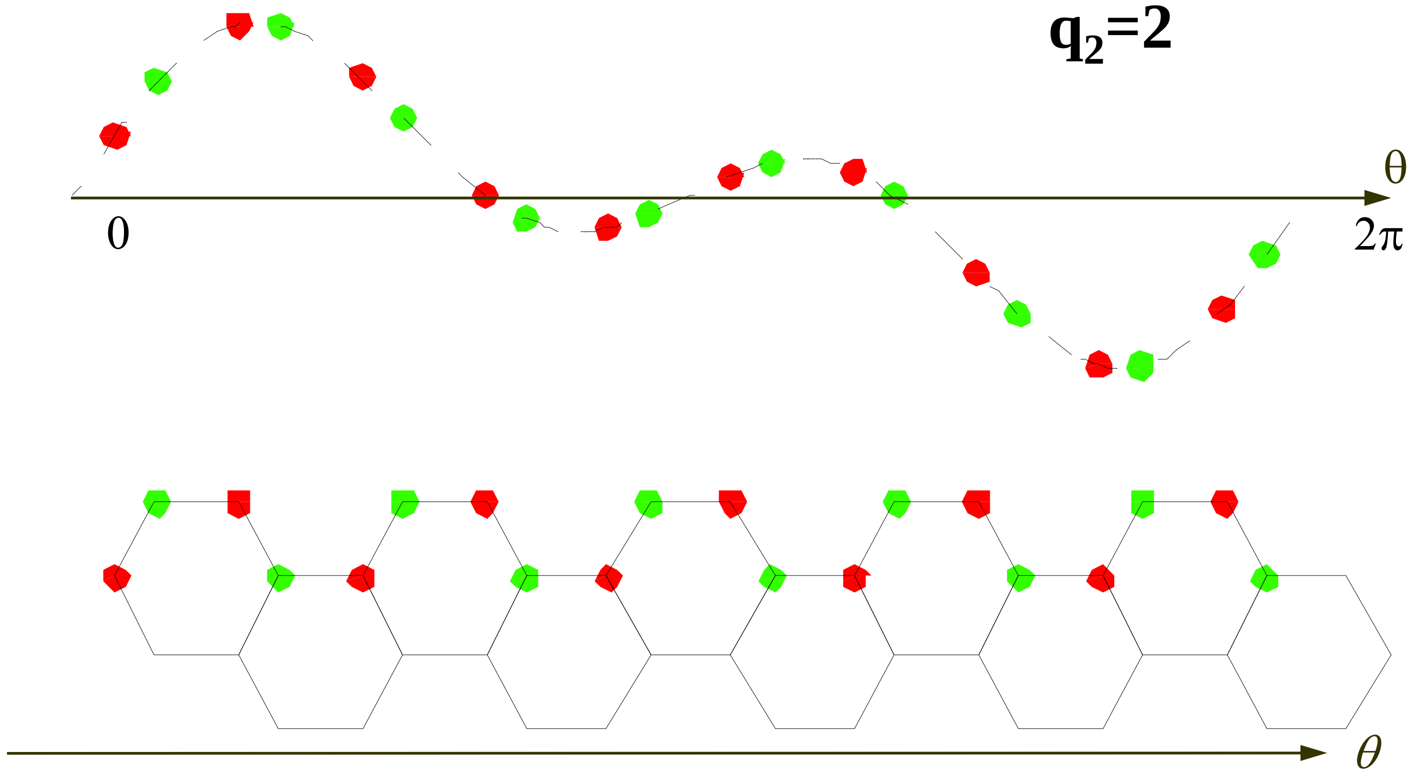


q=2n





$q_1=1$
$q_2=2$



Rule 2

Conservation law of angular quantum number m

$$|\pi\rangle \leftrightarrow |m_1\rangle \cdots |m_i\rangle \cdots |m_{\mu-1}\rangle \leftrightarrow |\pi^*\rangle \qquad m_{i+1} - m_i = \pm q$$

$$\mu_0 = \frac{2n}{\gcd(2n, q)} \quad = \text{odd}$$

- q =odd → μ_0=even, No M-S transition

→ Consistent with the case of uniform field and bending ($q=1$)

Direct coupling

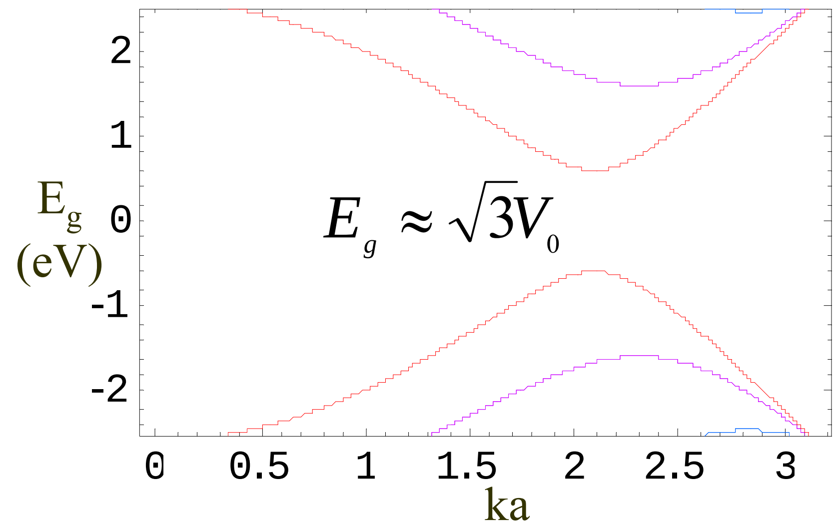
$$q = 2n$$

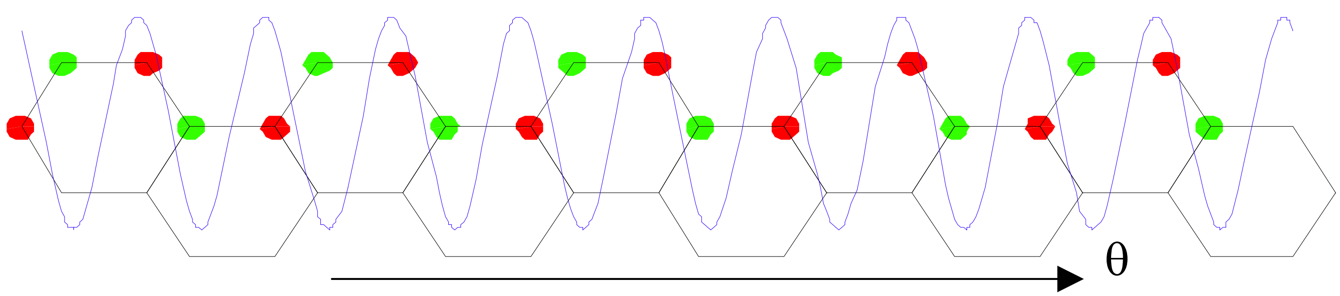
- Twisting
- Chem-/Bio- modification
- Strong local interactions

$$\delta(\theta) = \sum_m \exp[-im\theta]$$

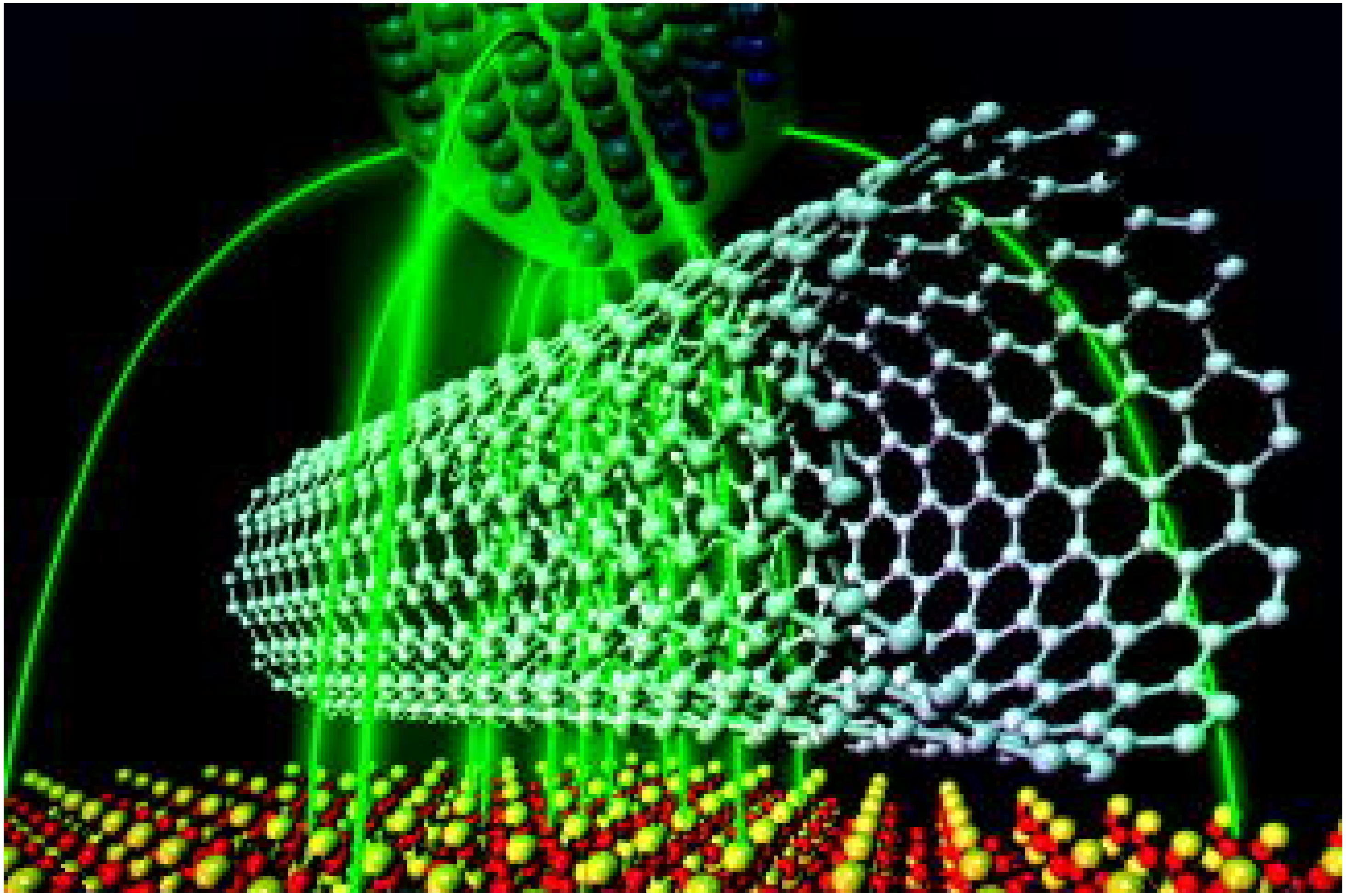
$$\mu_0 = \frac{2n}{\gcd(2n, 2n)} = 1$$

$$E_g = \sqrt{3}V_0$$





Possibility of a metallic field-effect transistor



S. V. Rotkin and K. Hess, *APL* **84**, 3139 (2004)

Indirect coupling

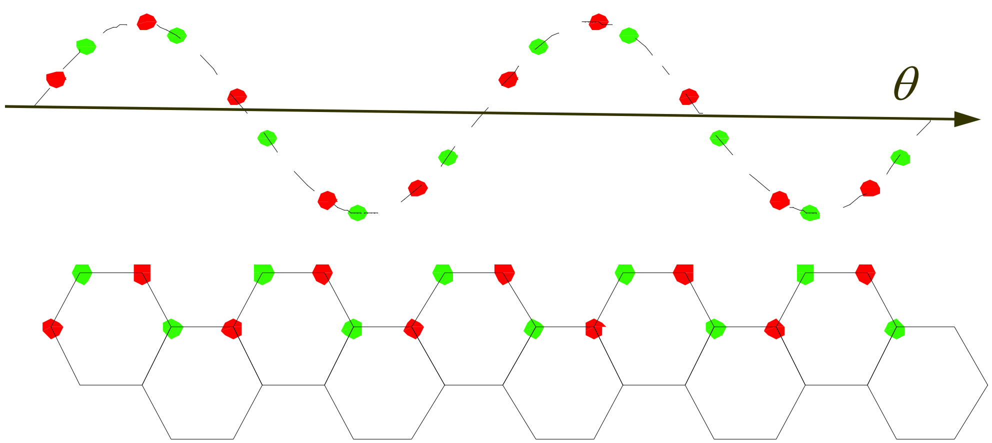
- Squashing
- Quadra-pole interaction
- Strong local interactions

$q = 2$

$$\mu_0 = \frac{2n}{\gcd(2n, q)} = n$$

- n=odd , e.g. (5,5)

$$E_g \propto V_0^{\ n}$$



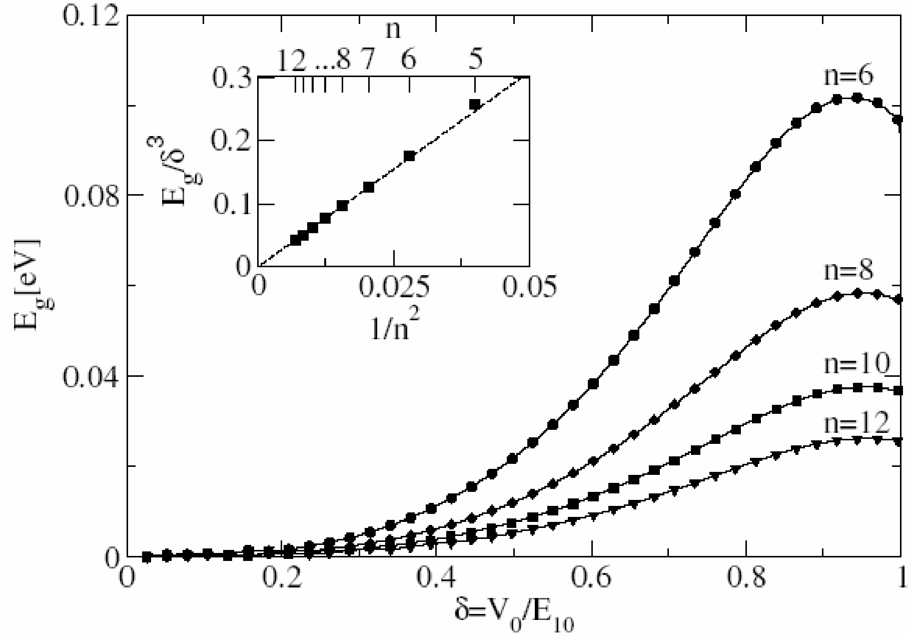
- n=even, e.g. (8,8) → no band gap from q=2 component of the perturbation
- Band gap in (8,8) case is due to local inter-layer interaction+ MSB

Mixed Fourier Components

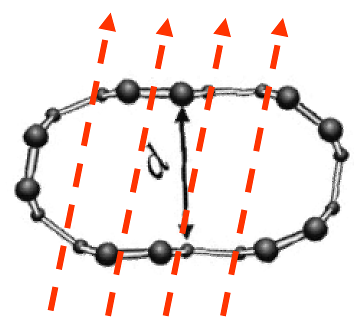
$$V = V_0 (\sin[\theta] + \sin[2\theta])$$

$$|\pi\rangle \overset{\delta m=1}{\leftrightarrow} |n \pm 1\rangle \overset{\delta m=2}{\leftrightarrow} |n \mp 1\rangle \overset{\delta m=1}{\leftrightarrow} |\pi^*\rangle$$

$$E_g \propto V_0^3$$



- Example:
  - Electric field (q=1)
  - +Mechanical deformation (q=2)



Summary

- Selection rules for M-S transition in armchair CNTs

  • Symmetry Breaking

  • Matching between the angular quantum number **q** of perturbation and the index number **n** of the armchair CNT

$$q \Leftrightarrow n$$

- Efficient ways of metal semiconductor transition by combining different types of perturbations