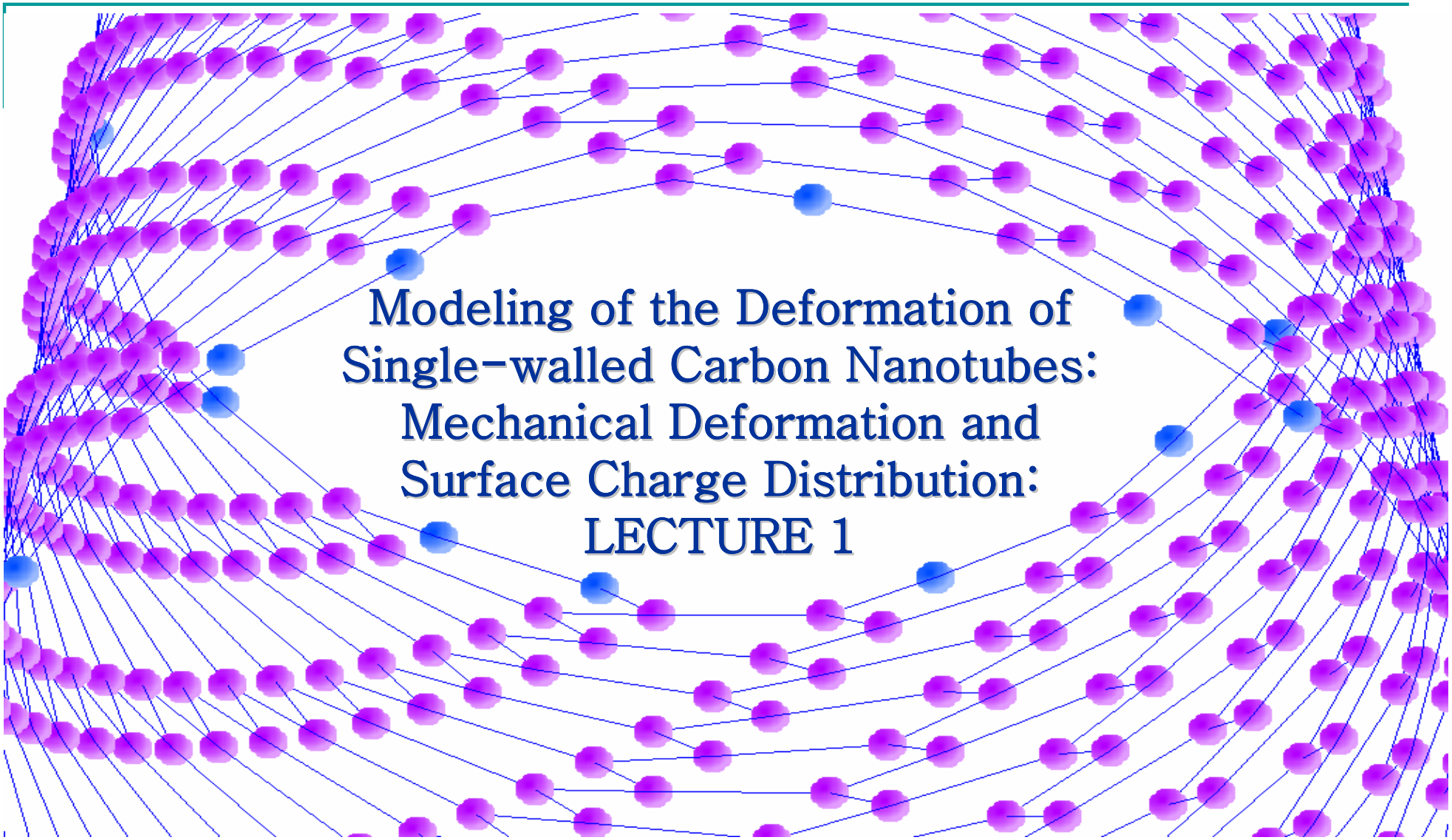


Modeling of the Deformation of Single-walled Carbon Nanotubes: Mechanical Deformation and Surface Charge Distribution: LECTURE 1

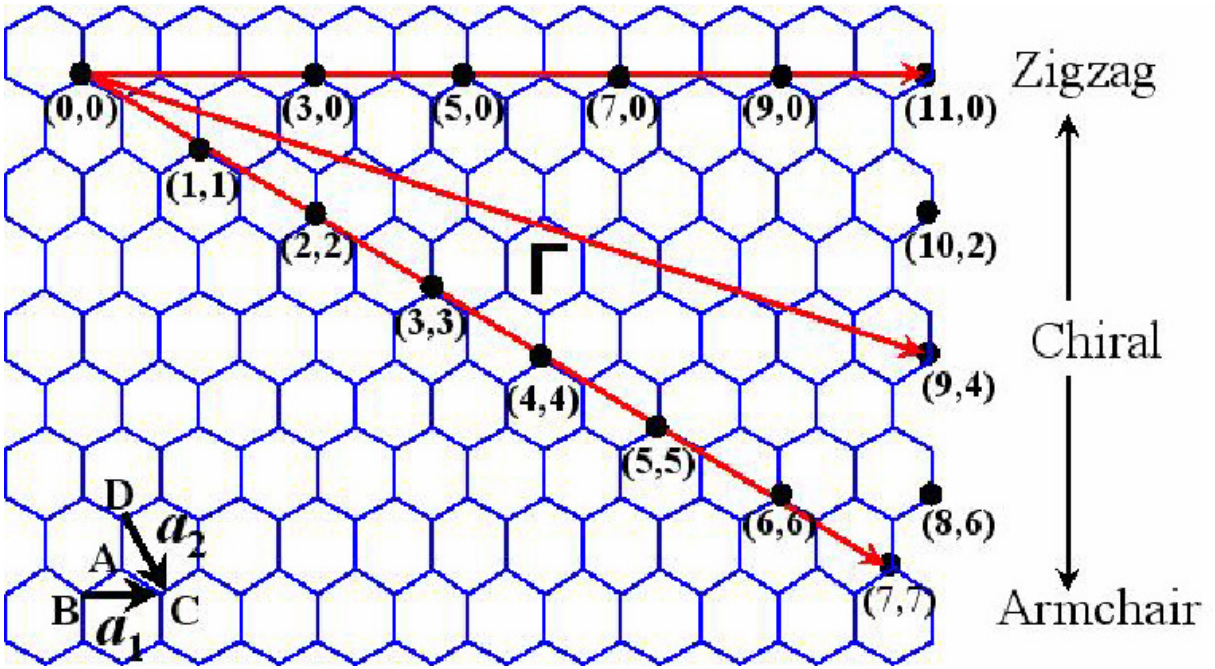
Subrata Mukherjee

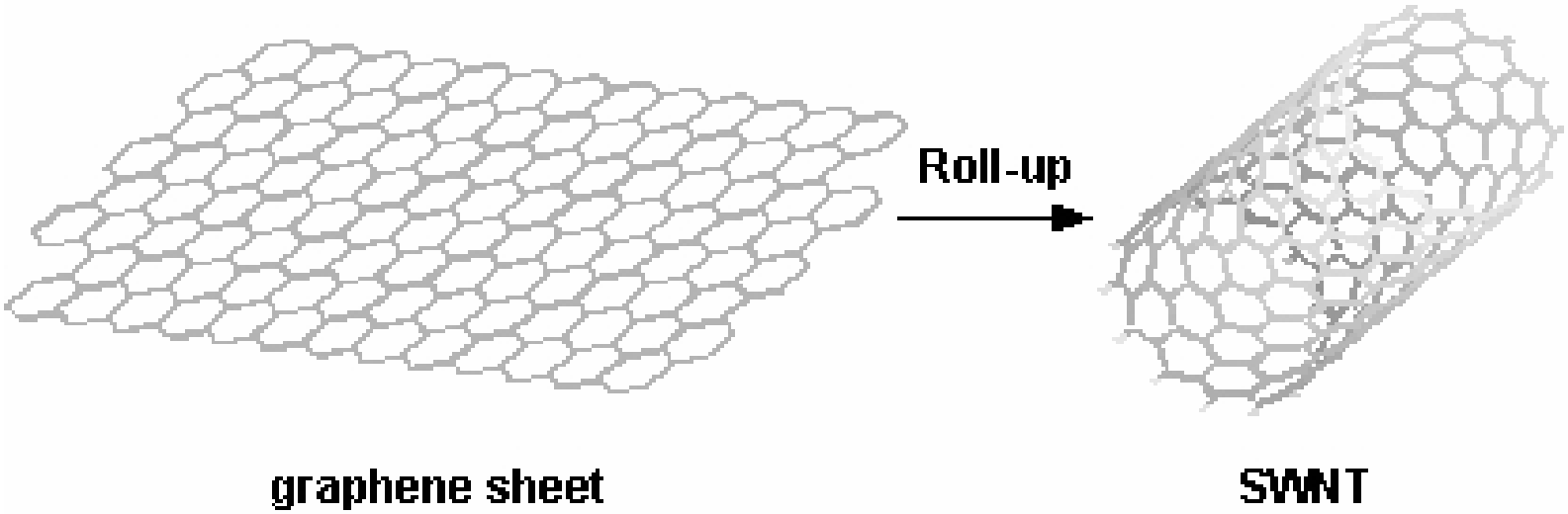
Cornell University, NY, USA

Introduction

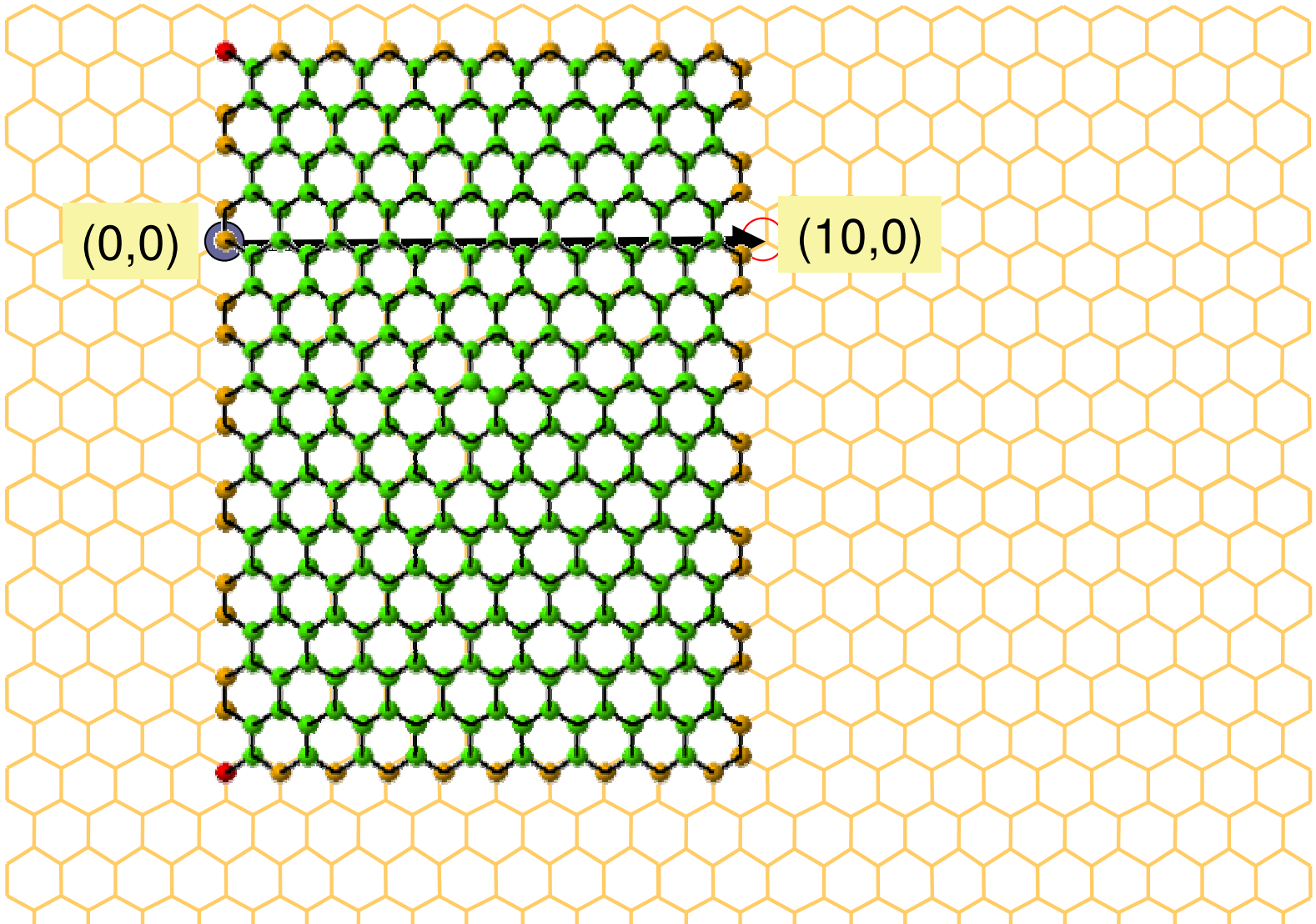
- Carbon nanotube (CNT) nomenclature:
  - Chirality – chiral, armchair and zig-zag CNTs
  - Single-walled nanotubes (SWNTs), nanotube bundles, multi-walled nanotubes (MWNTs)
- Experiments on CNT electromechanical oscillators
- Mechanical modeling approaches for CNTs:
  - Multi-scale paradigms
  - Overview of present work on SWNTs
- Course outline

Hexagonal Graphene Lattice (n,m)→ SWNT



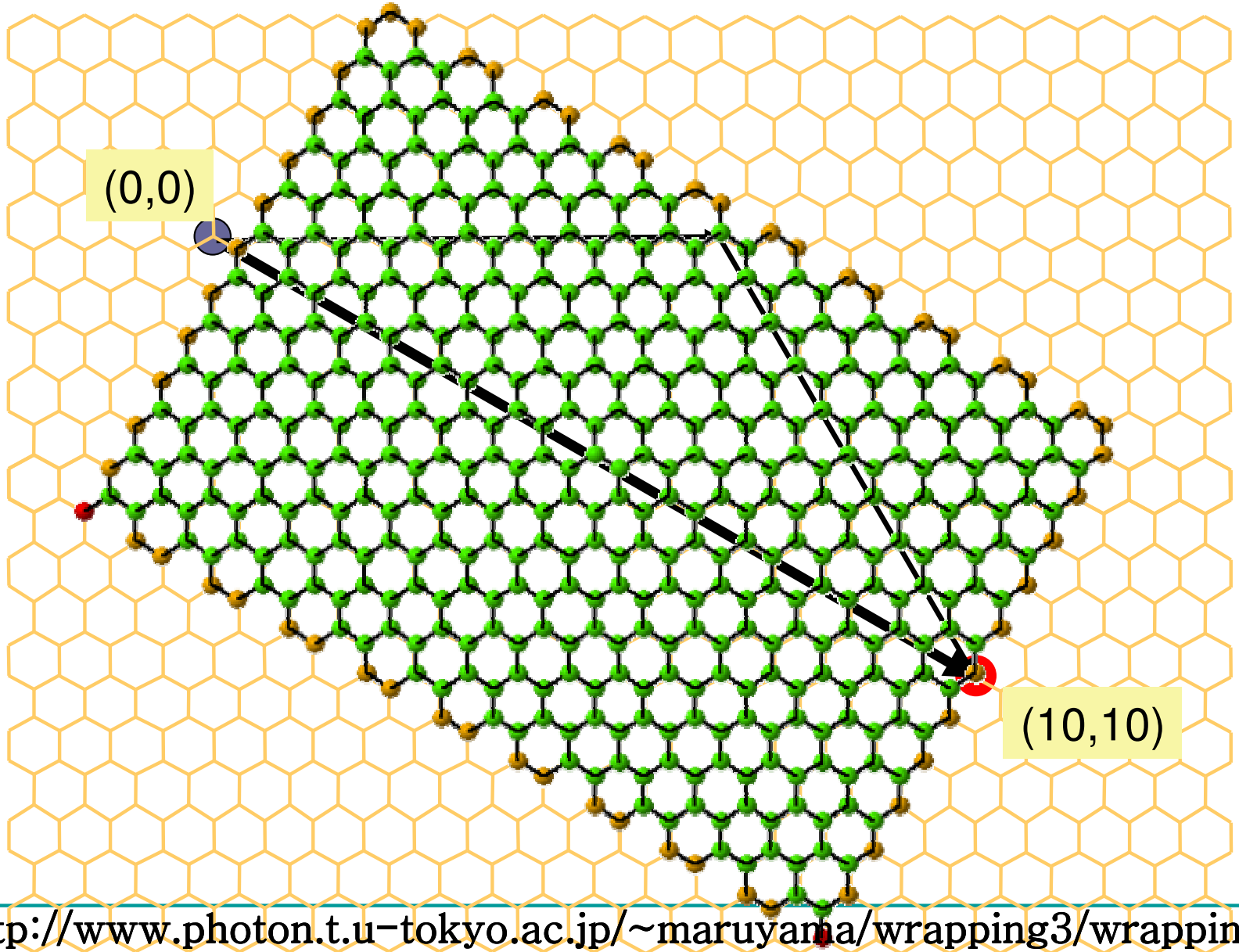


Wrapping (10,0): Zig-zag Nanotube



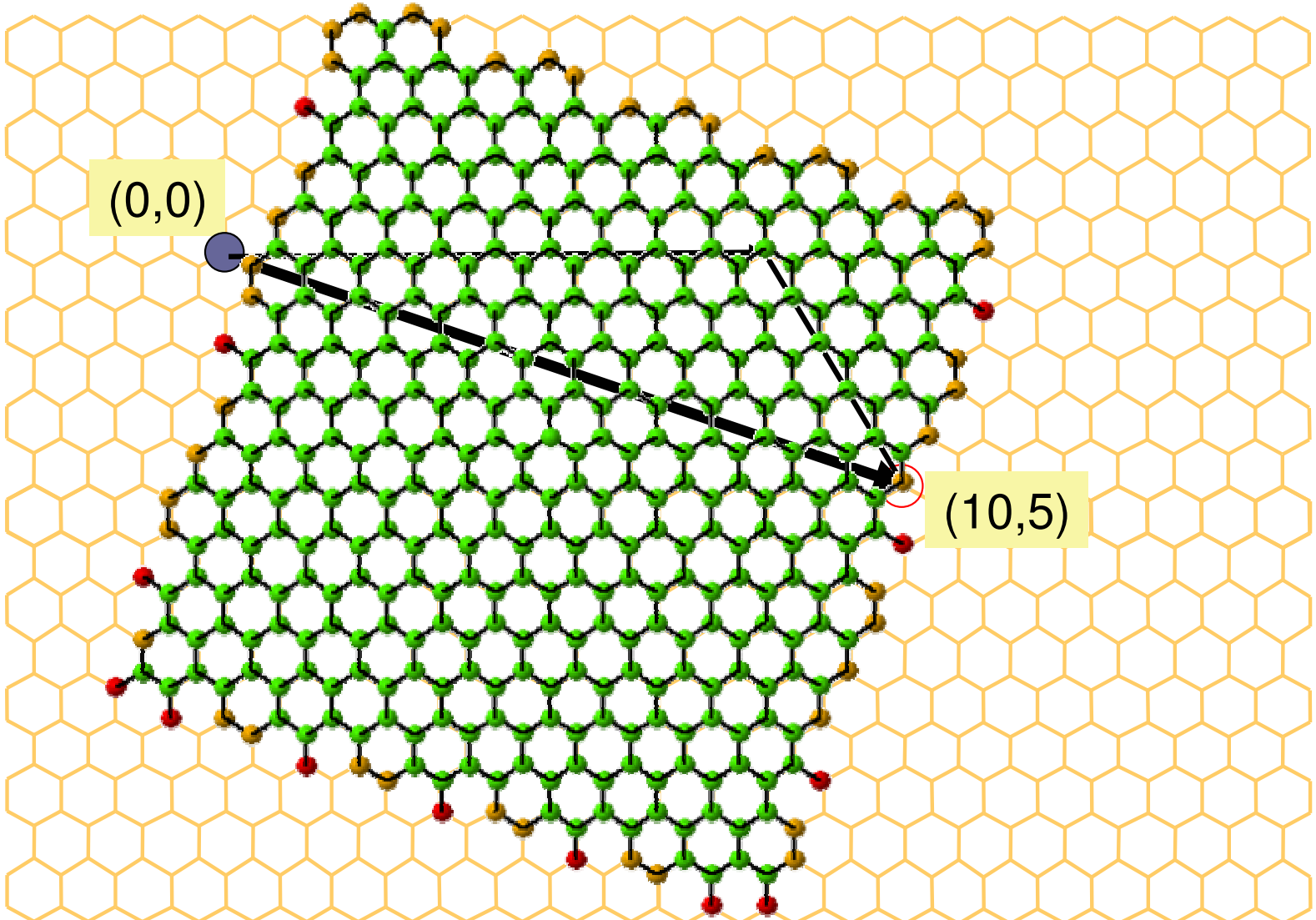
[http://www.photon.t.u-tokyo.ac.jp/~maruyama/wrapping3/wrapping.html]

Wrapping (10,10): Armchair Nanotube



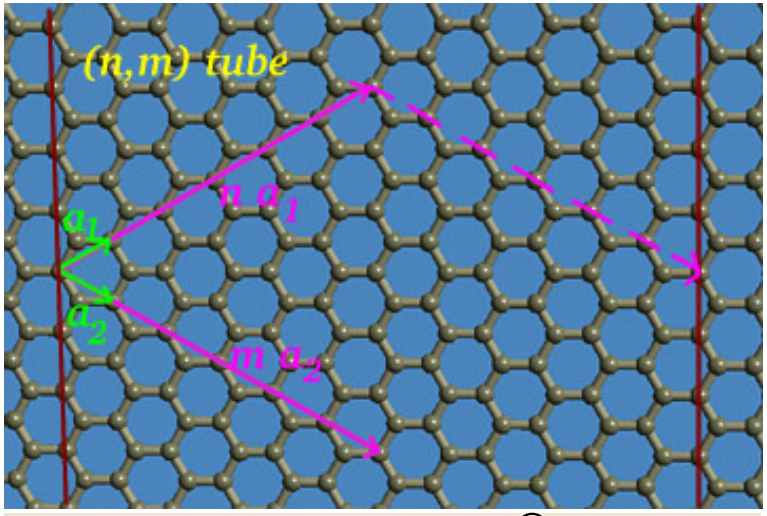
[http://www.photon.t.u-tokyo.ac.jp/~maruyama/wrapping3/wrapping.html]

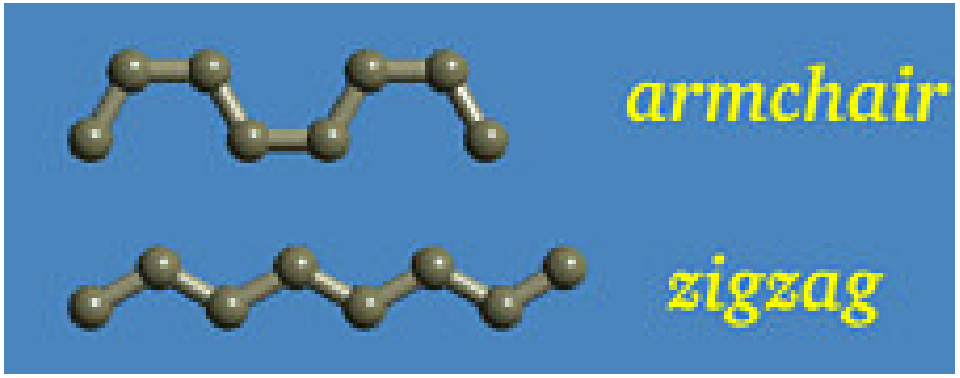
Wrapping (10,5): Chiral Nanotube

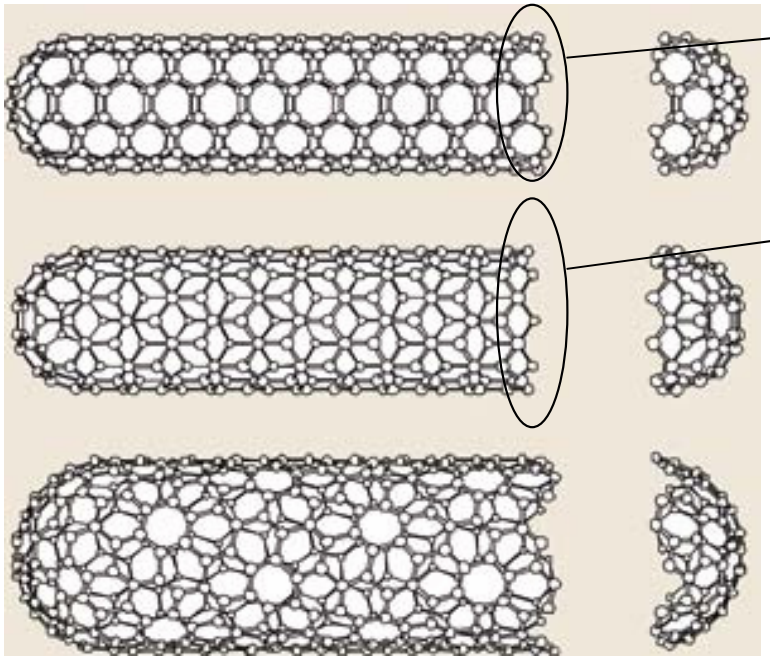


[http://www.photon.t.u-tokyo.ac.jp/~maruyama/wrapping3/wrapping.html]

Structural Configurations







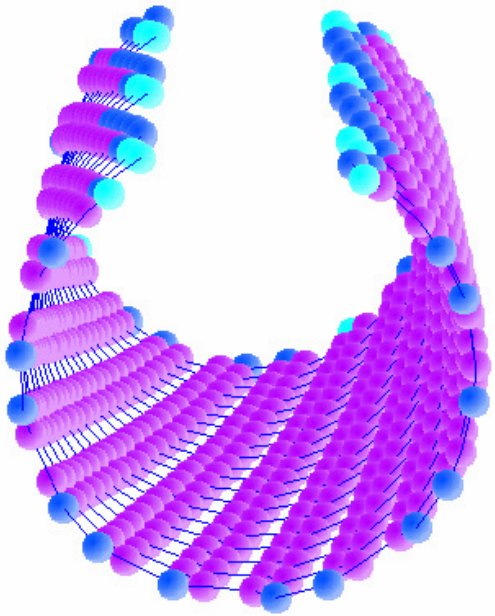
Armchair

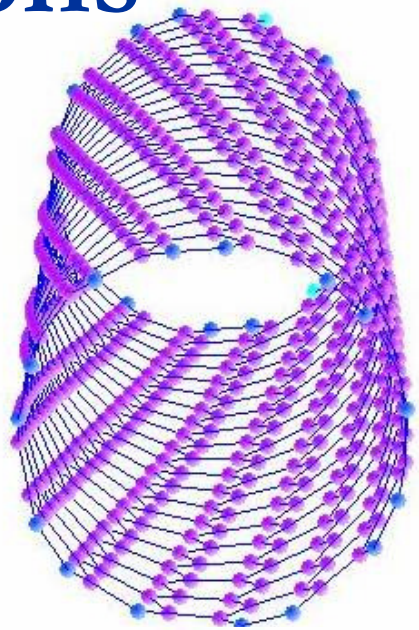
Zigzag

Chiral

Structural Configurations

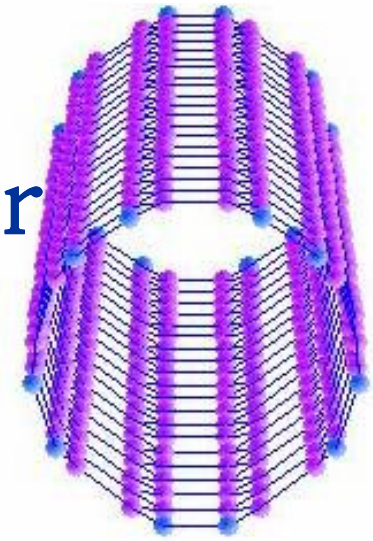
Roll-up



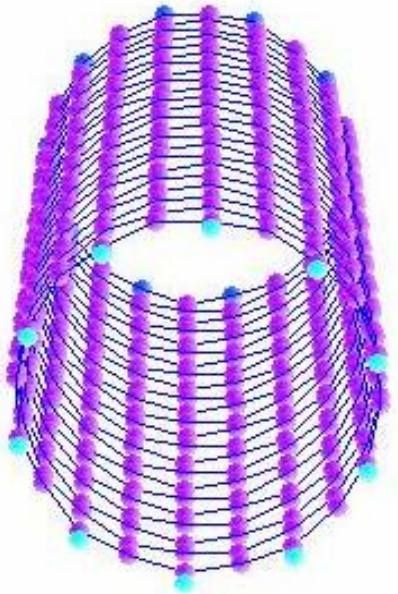


Chiral
(9,6)
Twisted!

Armchair
(5,5)

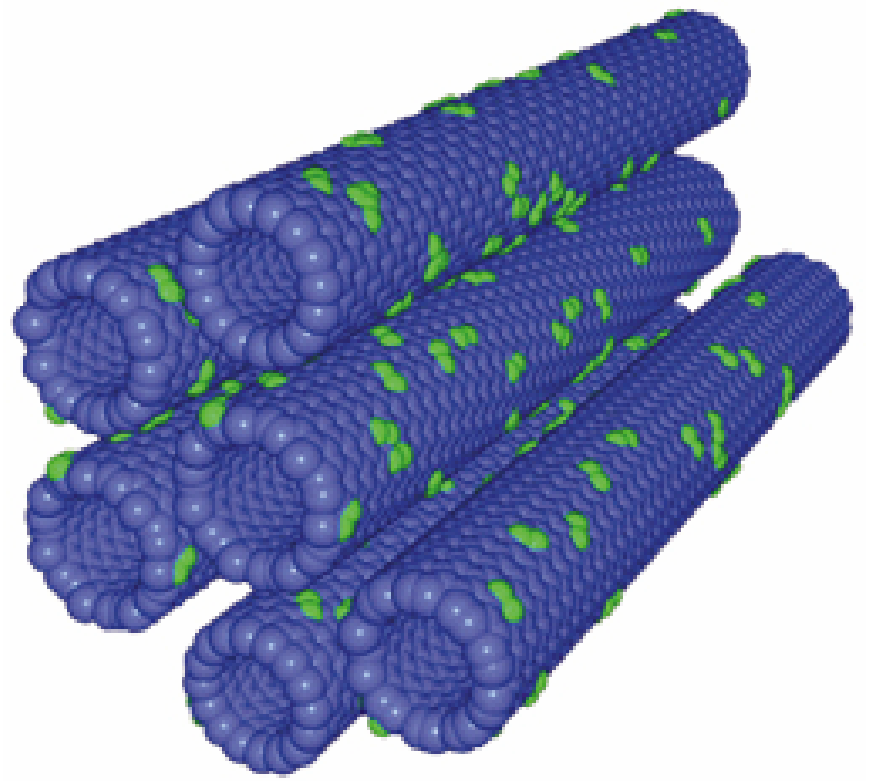


Symmetric!



Zig-zag
(10,0)

SWNT Bundles and MWNTs

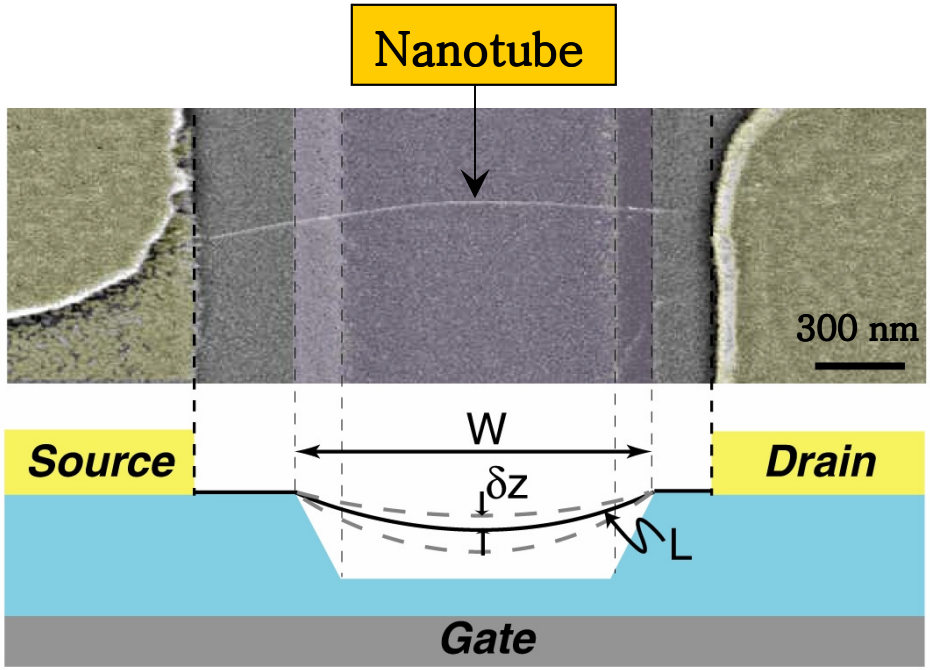


SWNTs are so O_2-sensitive that the absorption of even a few atoms of O_2 (shown in green) can change semi conducting tubes into conductors.

The controlled and reversible telescopic extension of MWNTs as shown in the computer graphic [above], could lead to virtually frictionless nanoscale linear bearings and constant-force nanosprings.

Ref: http://www.lbl.gov/Science-Articles/Research-Review/Magazine/2001/Fall/features/02Nanotubes.html

Nanotube Oscillators: Coupled Electro–mechanics



Sazonova et al., Nature, Vol. 431, 2004, pp. 284–287.

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Gate Voltage:
DC: nanotube tension, natural frequency
AC: nanotube excitation

- Widely tunable resonance frequencies
- Ultra sensitive force and mass detection

Present Work: Constitutive model for nanotube mechanical deformations

Mechanical Modeling Approaches for CNTs

Fully Atomistic Descriptions

- Empirical interatomic potential: Tersoff-Brenner multi-body potential for hydrocarbons
- Ab initio approaches: Approximate solutions to the many-body Schrödinger equation for periodic solids – Hartree-Fock, Tight-binding (LCAO), Density functional theory

MULTISCALE METHODS

Fully Continuum Description

- Beam theories – Euler-Bernoulli, Timoshenko
- Thin shell theory
- Need to assume cross-sectional area, wall thickness and isotropic Young's modulus from experiments/atomistic calculations

Multi-scale Modeling Paradigms - I

- **Direct coupling methods**: Decompose physical domain into atomistic, continuum and interface regions (where information is exchanged between scales).

- **Bottom-up methods**: Coarse-grain atoms and equations to equivalent macro-scale equations – Coarse-grained molecular dynamics (MD), multi-grid bridging approach.

- **Top-down methods**: Solve continuum equations by extracting constitutive laws from underlying atomistic descriptions – quasicontinuum (QC), bridging-scale method, heterogeneous multi-scale method.

Present work: Top-down approach

Multi-scale Modeling Paradigms - II

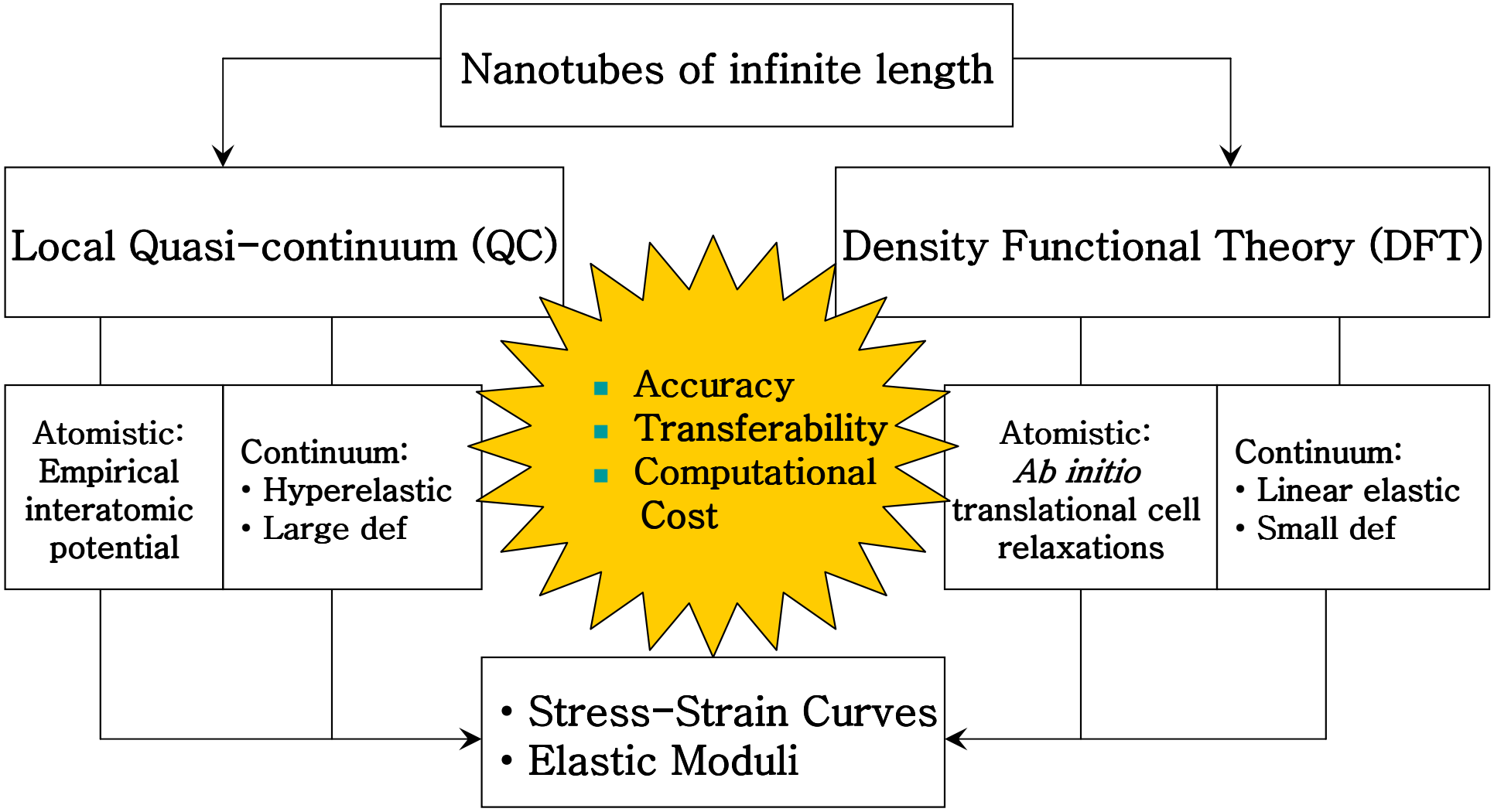
- **Hierarchical methods**: Small scales depend on large scales in some predictable way; based on assumption of homogeneous lattice deformations – more effective for elastic single-phase problems, difficulties in modeling lattice defects and dislocations.

- **Concurrent methods**: Appropriate model solved at each length scale **simultaneously**; inter-scale dependence not pre-assigned; more relevant for inhomogeneous lattice deformations, fracture, multi-phase materials, nanofluidics; challenges – (a) how to separate scales (b) what is the mechanism to couple scales.

- **Multi-scale boundary condition methods**: Employed within concurrent methods to eliminate artificial "handshake" region between scales, result in smooth FE-MD transition.

Present work: Hierarchical approach

Mechanical Modeling Approaches: Present work

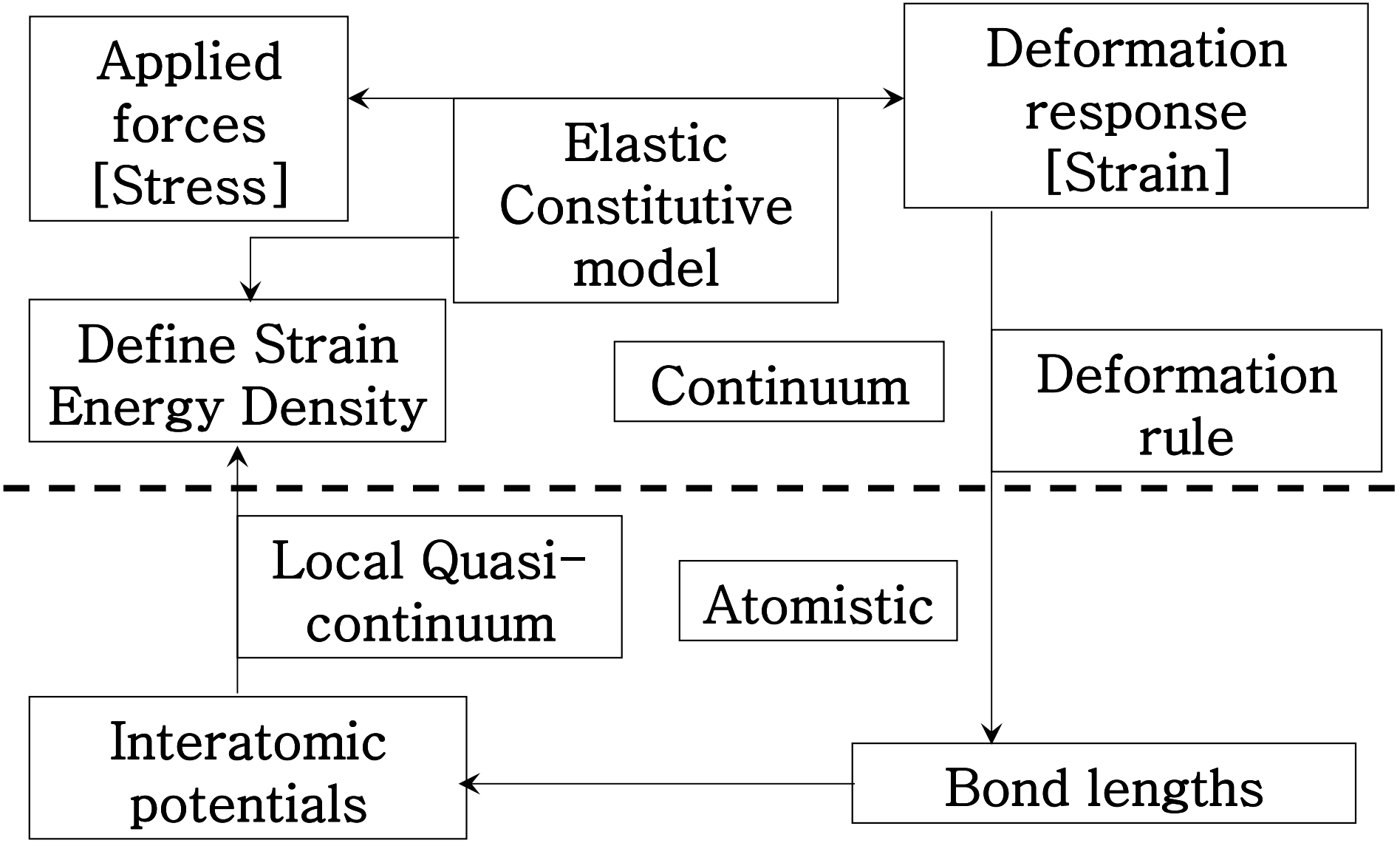


QC vs. DFT: Preliminary Comparison

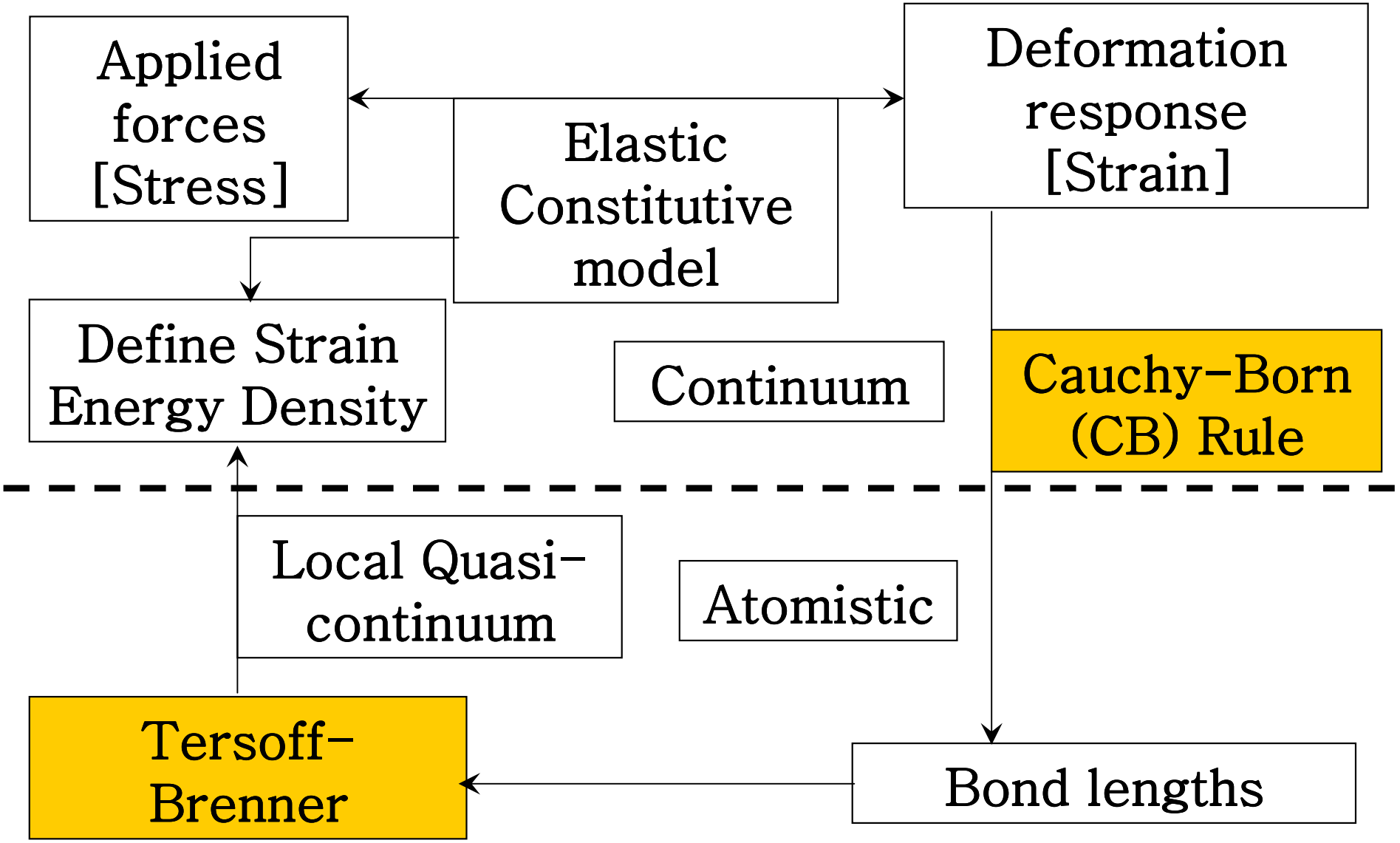
Local QC with Empirical Potential	*Ab initio*: DFT
☺ Closed-form expressions for interatomic energies: ■ Analytic derivatives ■ Computationally efficient ■ Can treat large number of atoms	☹ Numerical approach: ■ Curve fit to numeric data ■ Computationally expensive ■ Restricted size of atomic system
☹ Contains experimentally fit parameters	☺ No experimentally fit parameters
☹ Accuracy limited by choice of potential	☺ Accuracy capable of systematic improvement

- Choose appropriate approach depending on application requirement
- Present work: Compare the 2 approaches in estimating continuum constitutive laws

Local QC Approach: Overview



Local QC Approach: Overview



Course Outline

- Coupled extension and twist of SWNTs using local QC approach with Tersoff–Brenner interatomic potential:
  - Kinematic coupling between extension and twist of CNTs:
    - Comparison of classical CB rule with a direct deformation map and motivation for the exp CB rule
    - Extension of exp CB rule for inhomogeneous deformations
    - Kinematic coupling revisited using extended exp CB rule
  - Stress–strain curves
  - Elastic moduli – Young's and shear moduli
- DFT *ab initio* approach:
  - Need for an *ab initio* approach
  - Simulation set–up details and numerical results: Young's modulus
- Charge distribution on the surface of conducting SWNTs:
  - Line model for the boundary element method (BEM)
  - Numerical simulations for charge per unit length along tube and charge density on tube surface