3rd NASA-NIST Workshop on Nanotube Measurements
26-28 September 2007, Gaithersburg, MD

Atomic-level characterization of carbon nanotubes

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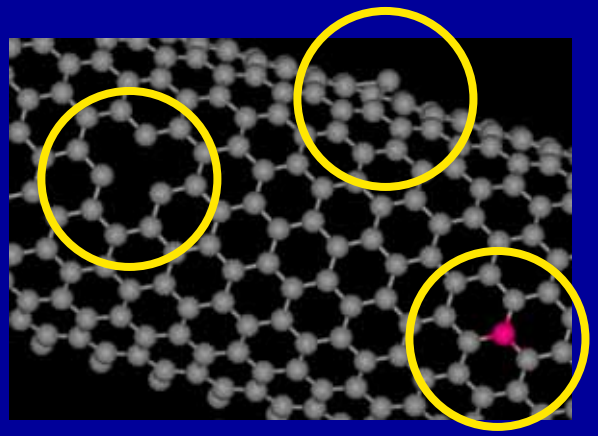
As any other material, the carbon nanotube should not be regarded as perfect (defect-free).

Defects and impurities, Chirality, dopant

Physical and chemical properties



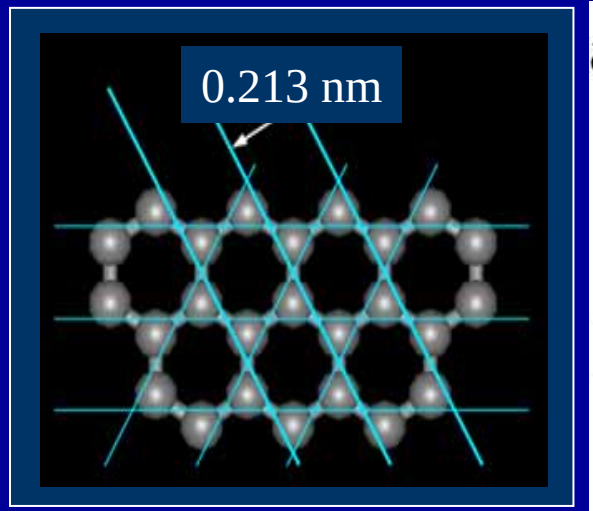
Relationship between atomic structures and properties should be precisely understood.

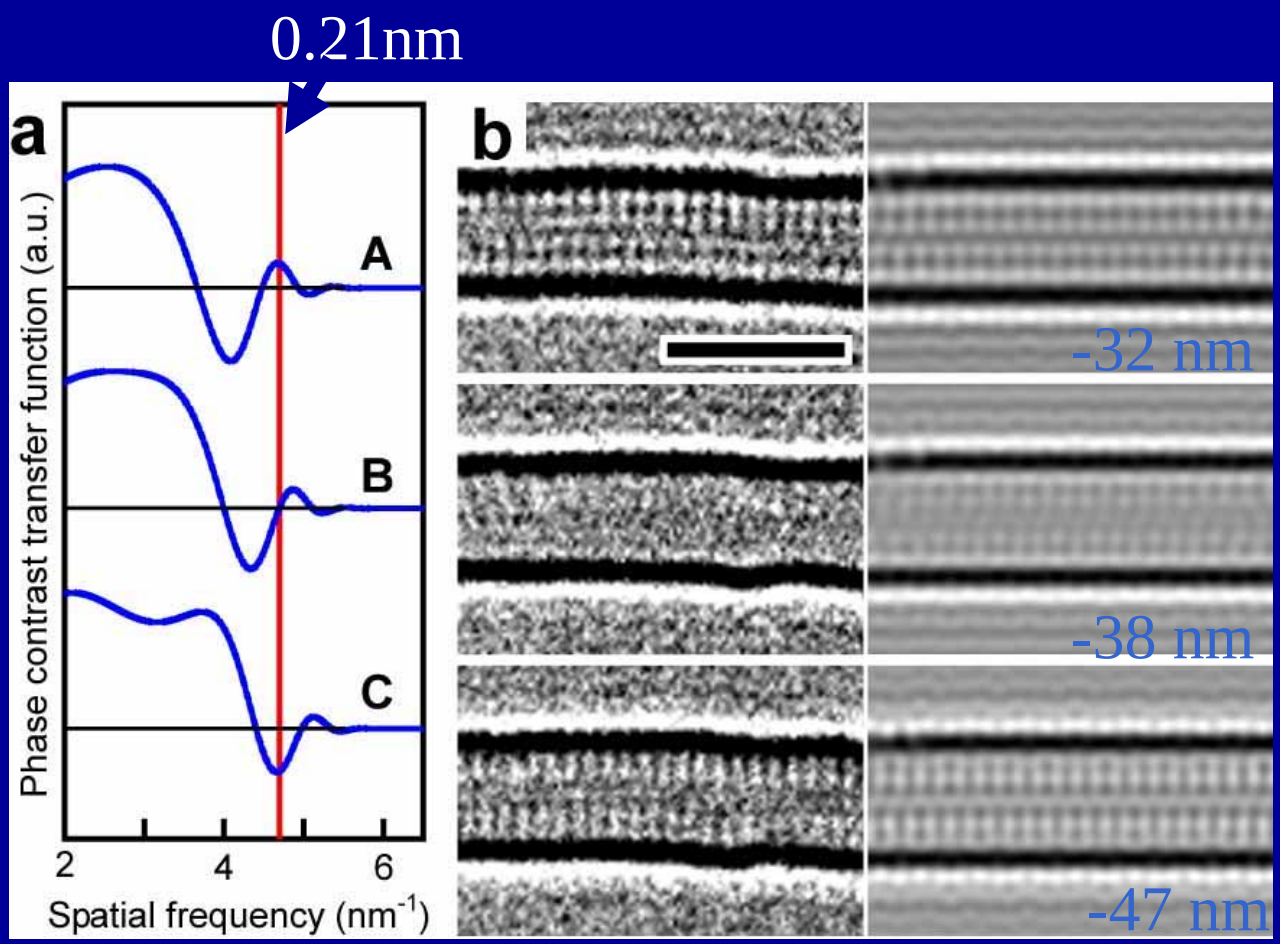
Characterization techniques developments of TEM,

Reproducibility, device stabilities,

Practical applications in industry

The minimum of HR-TEM theory (an advantage of Cs-uncorrected TEM)





At 120 kV
Cs=0.45 mm

Y. Sato

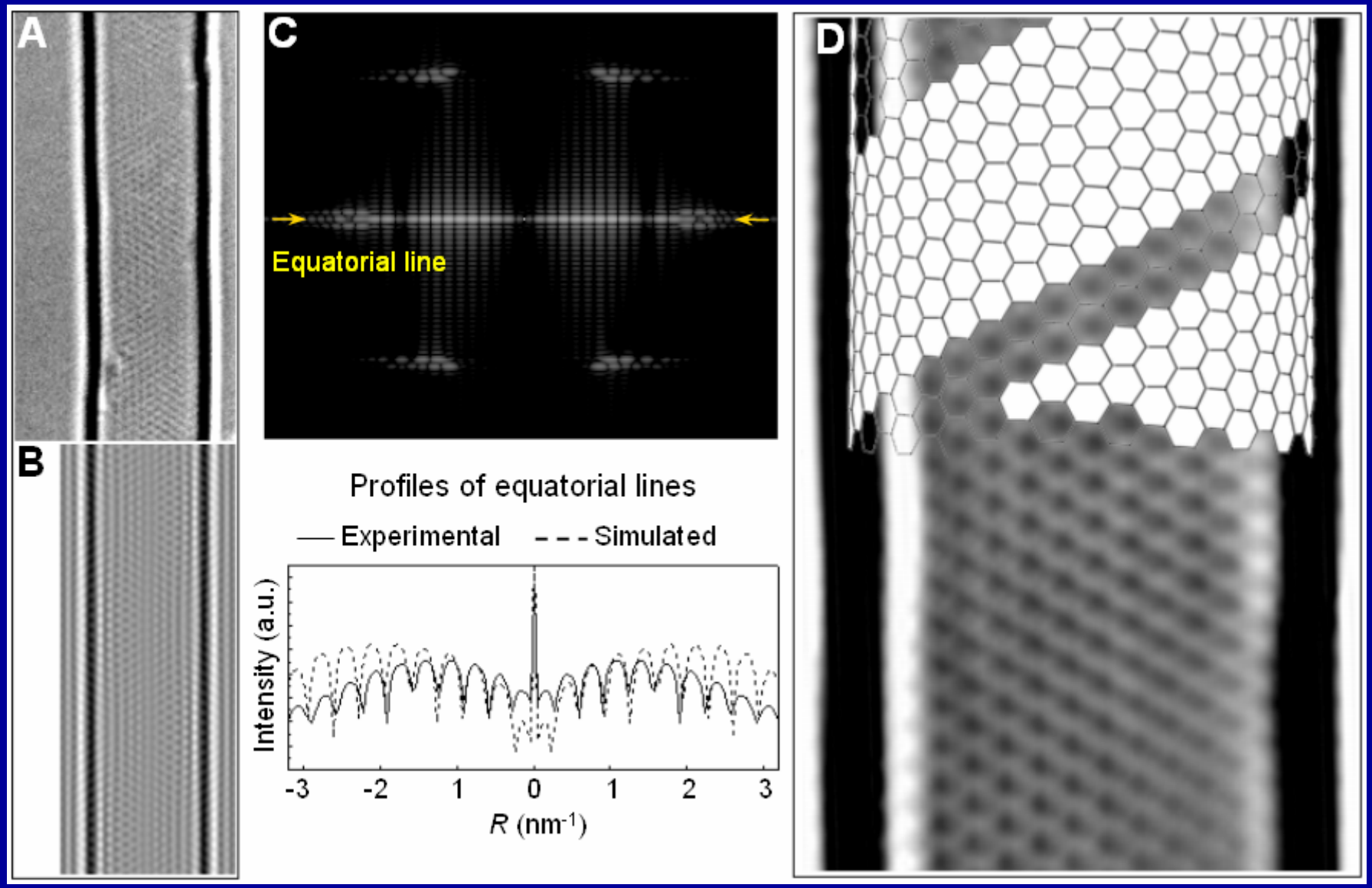
Chirality and handedness relationship in DWNT

Hashimoto at al., PRL (2005)

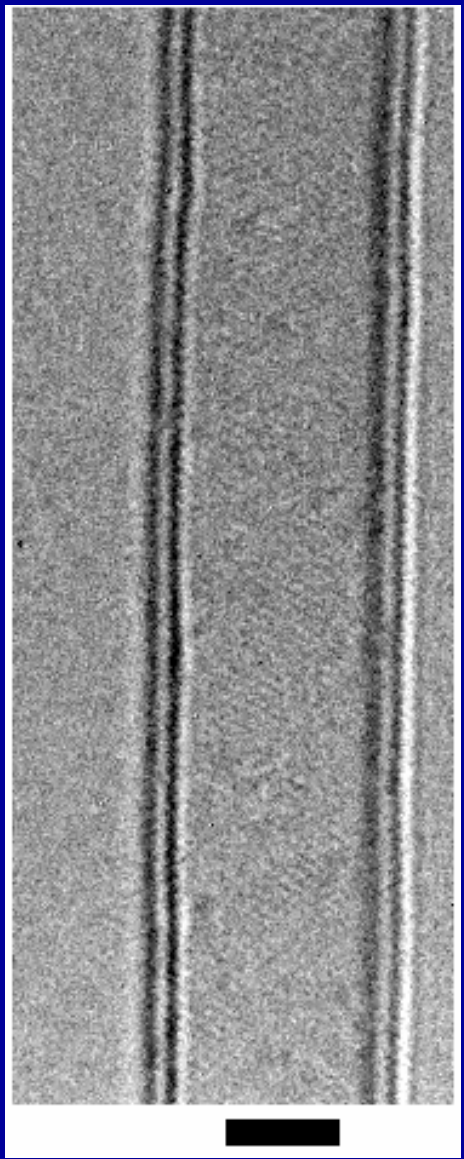
Zhu et al., CPL (2005)

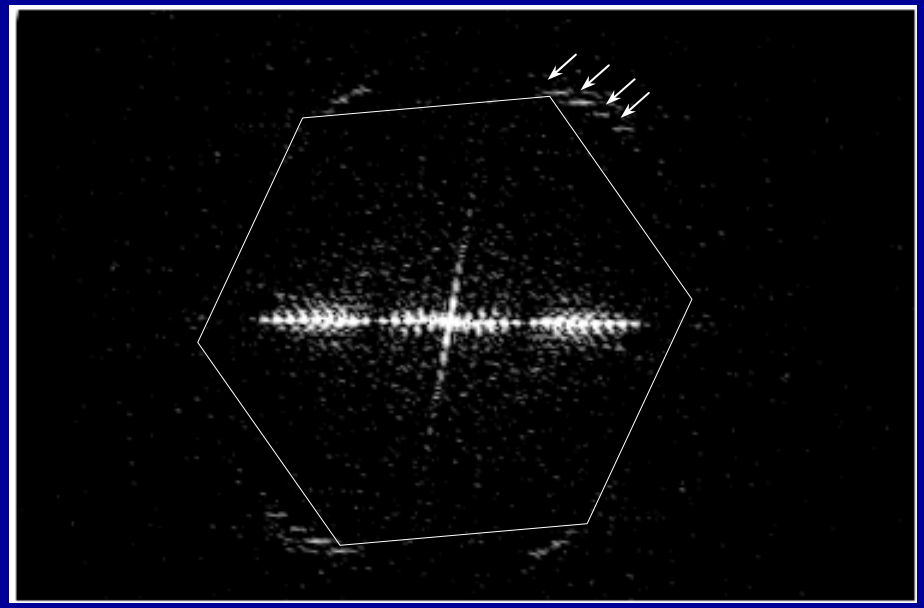
Liu et al., PRL (2005)

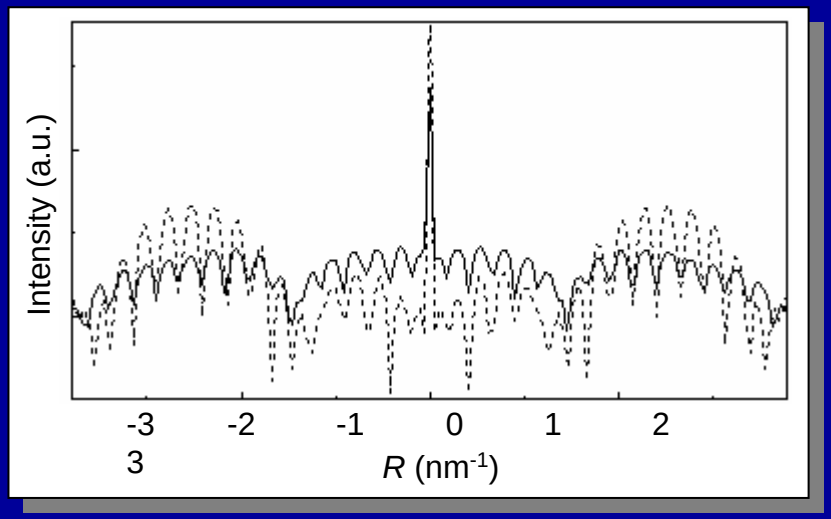
Direct observation of graphen network in the case of SWNT

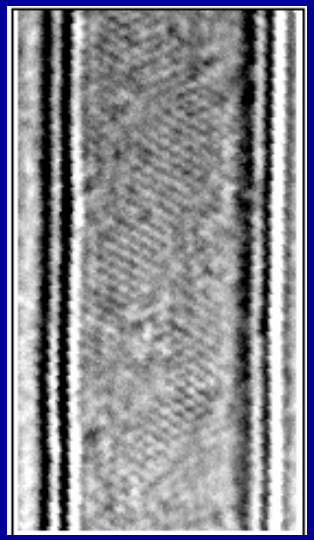


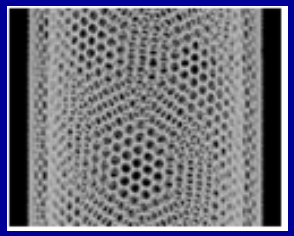
Double-walled tube

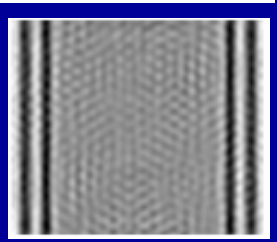




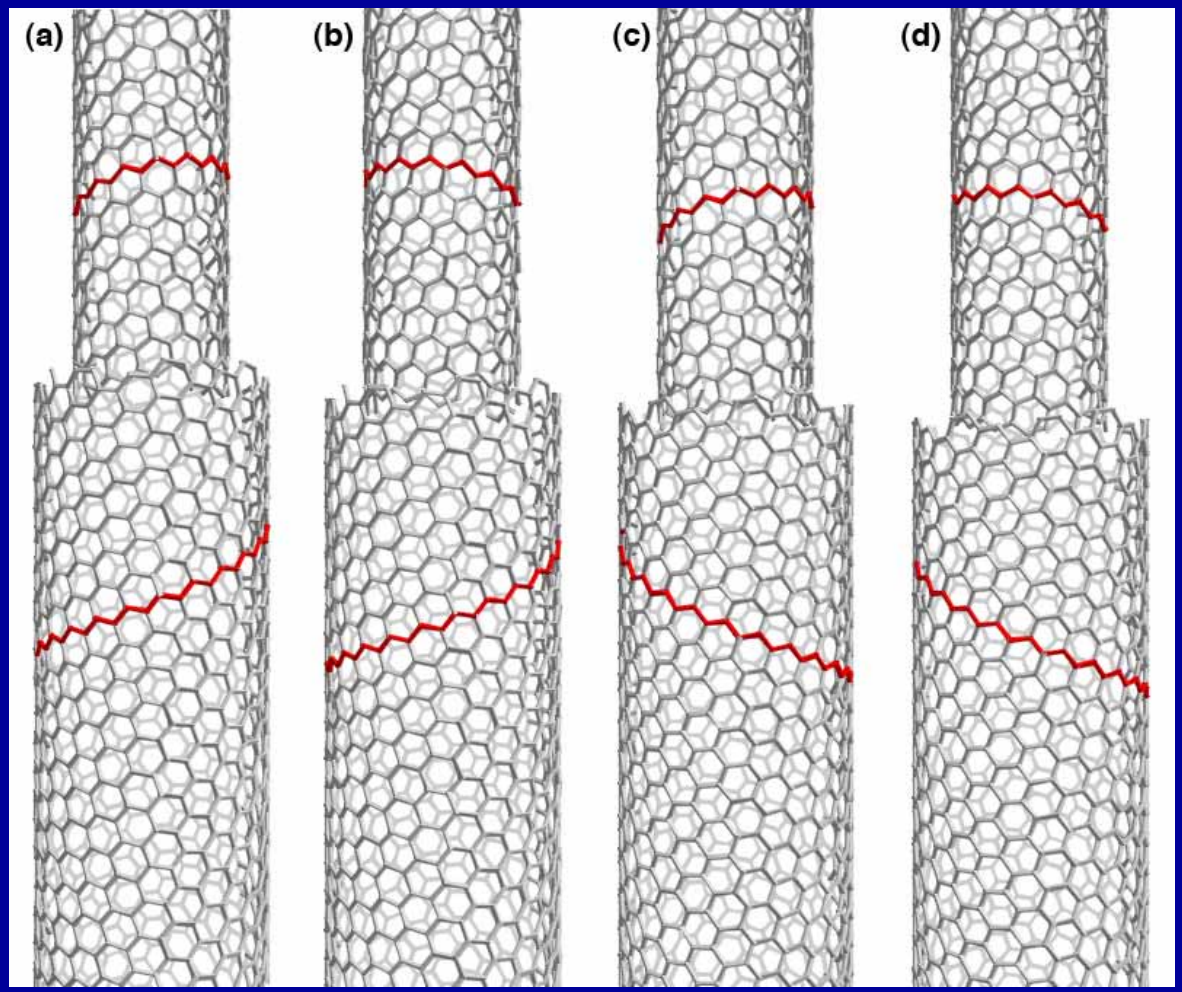




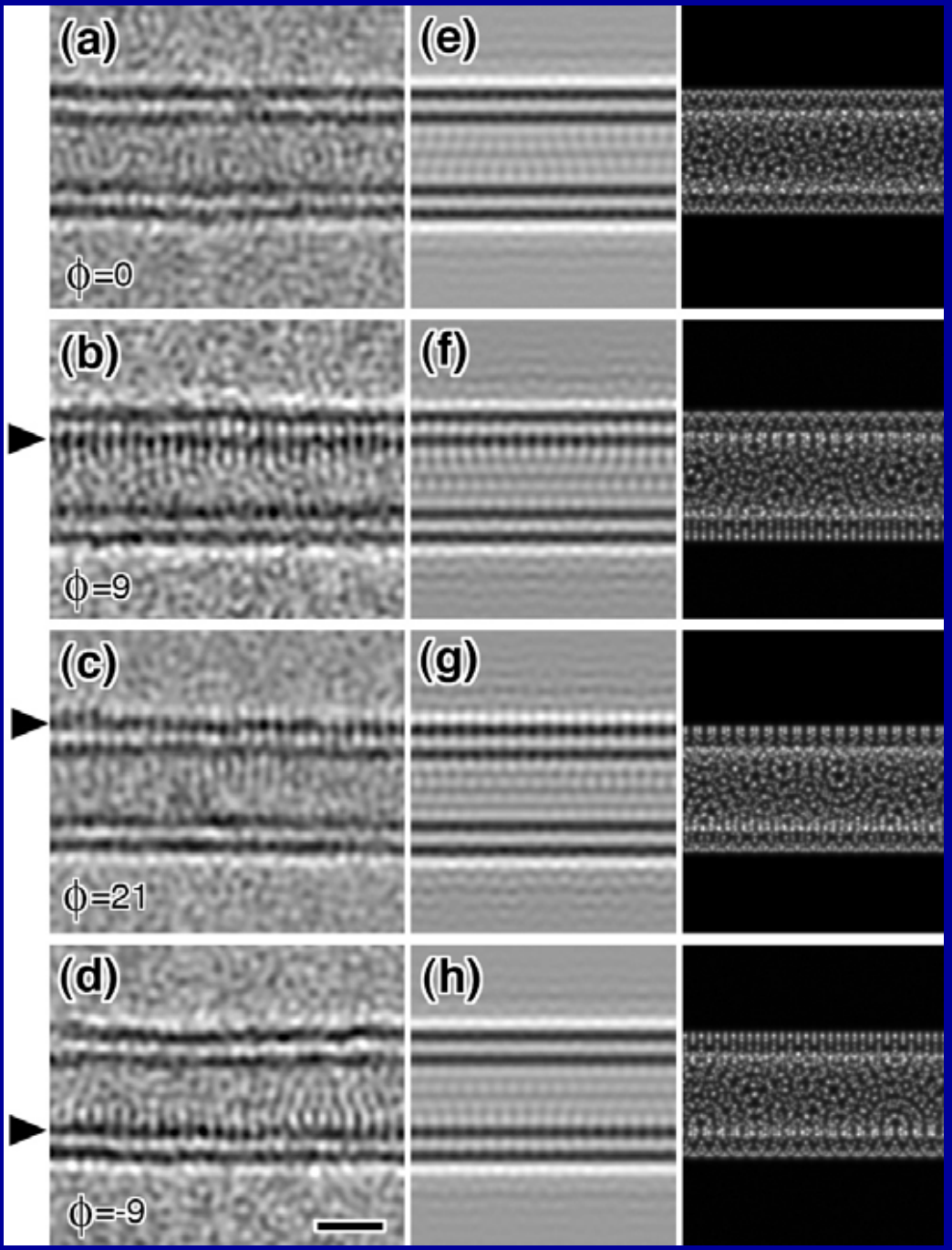


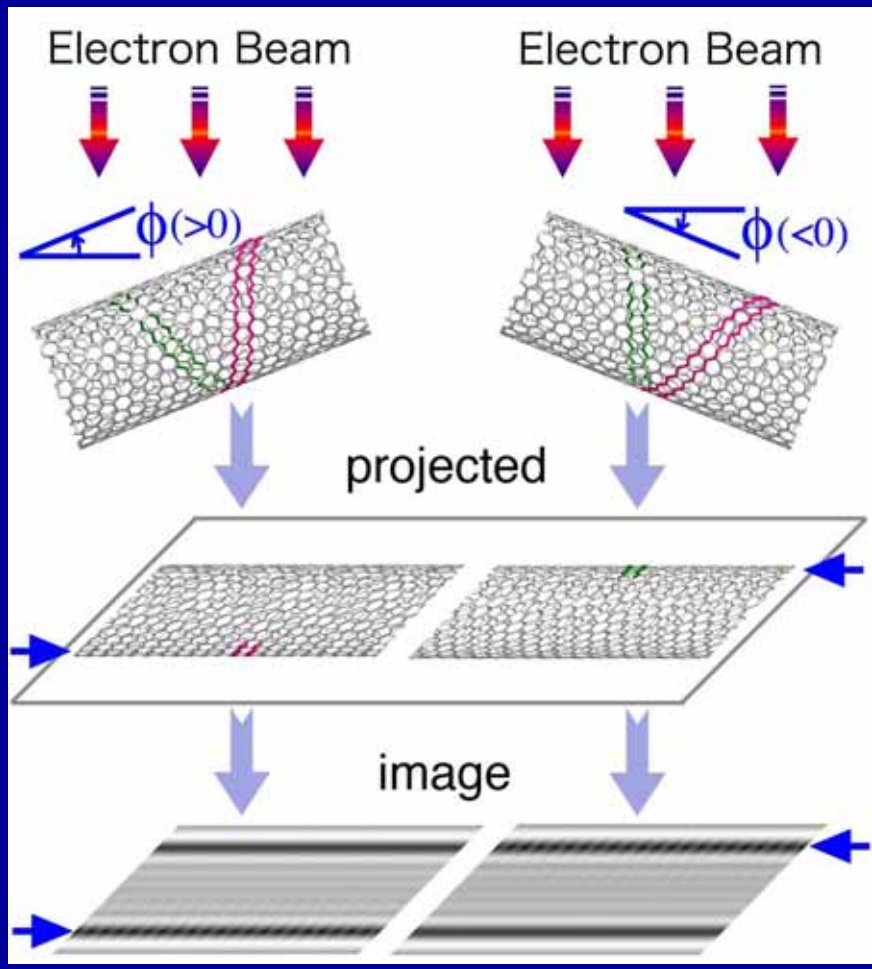


Four combinations of different optical isomers in a chiral DWNT

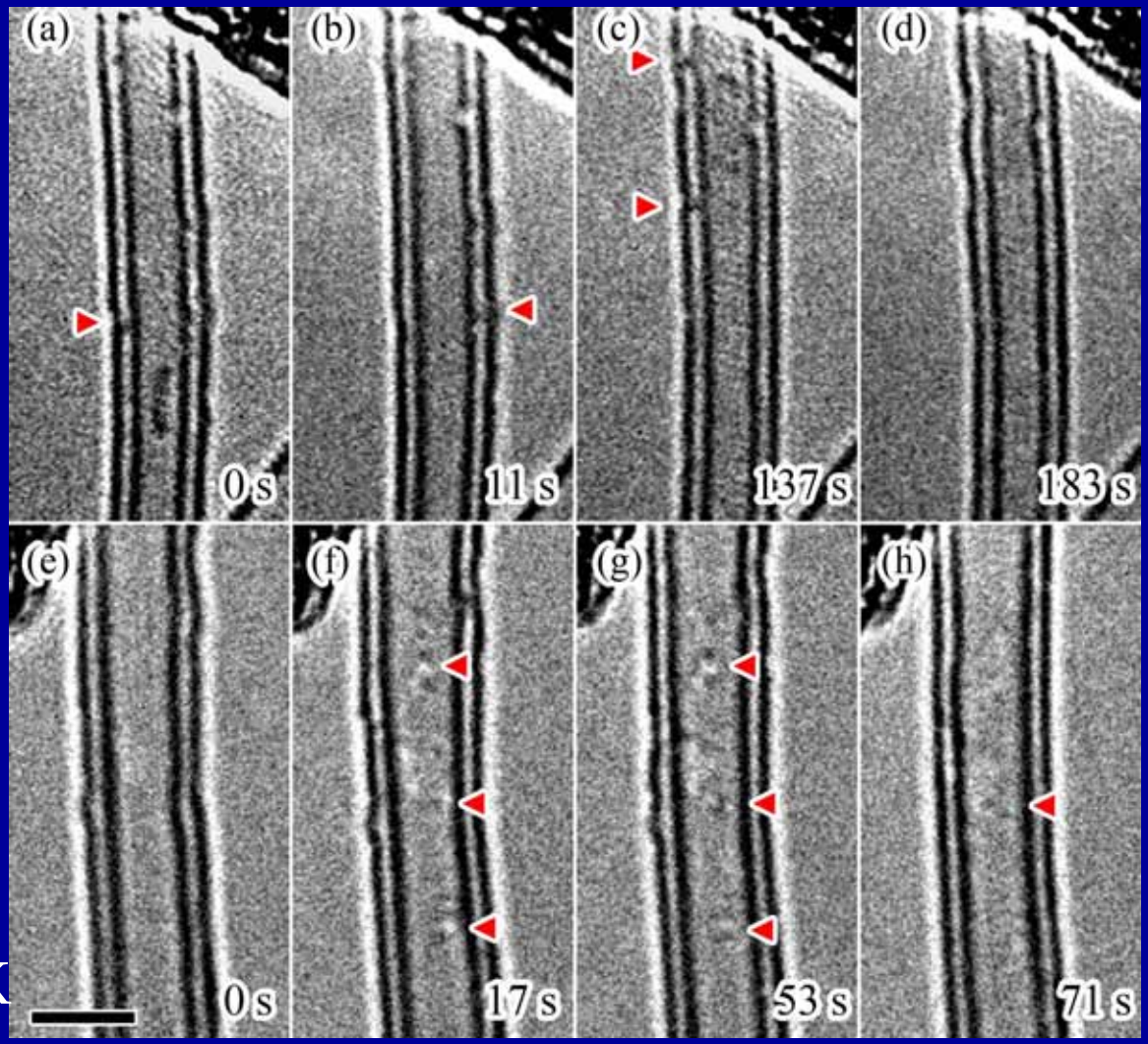


(a) (14, 3)@(17, 10)
(b) (3, 14)@(17, 10)
(c) (14, 3)@(10, 17)
(d) (3, 14)@(10, 17)

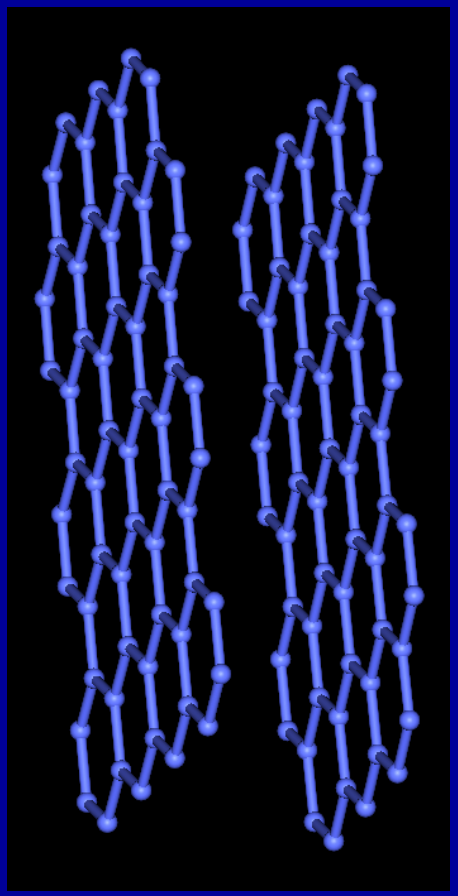

(a)
(e)
ϕ=0
(b)
(f)
ϕ=9
(c)
(g)
ϕ=21
(d)
(h)
ϕ=-9


Electron Beam
Electron Beam
ϕ(>0)
ϕ(<0)
projected
image

Formation and annihilation of Frenkel pair defects (the inter-layer defects)



523K



A single interstitial and vacancy pair (I-V pair)

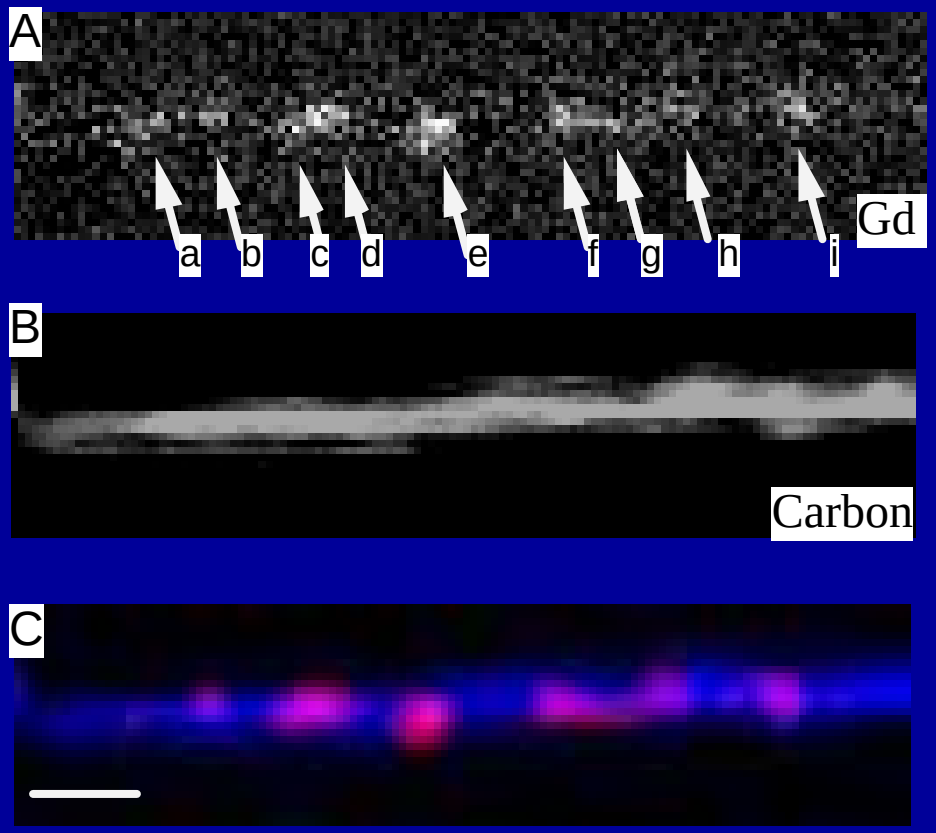
Visualization of dopant atoms, K, Cs, Iodine and $FeCl_2$

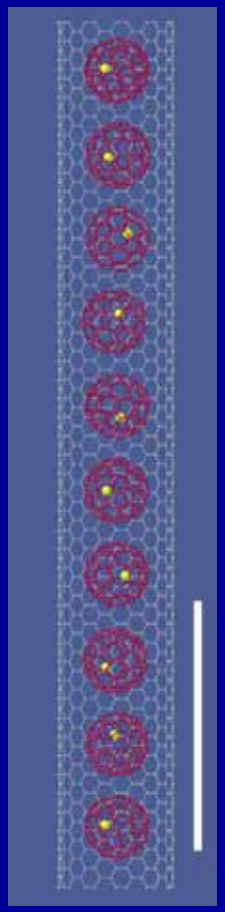
Guan et al., PRL (2005)

Sato et al., (unpublished)

Single dopant atom detection in SWNT

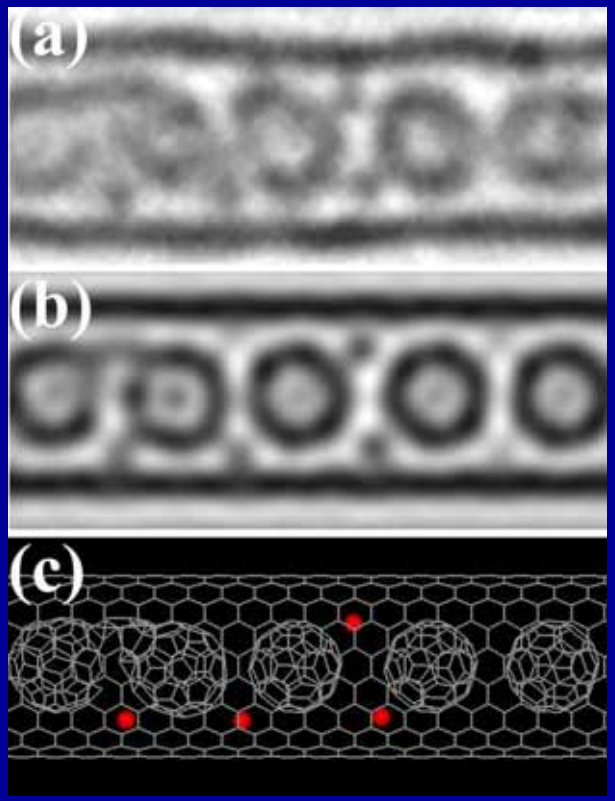
Science **290** (2000) 2280

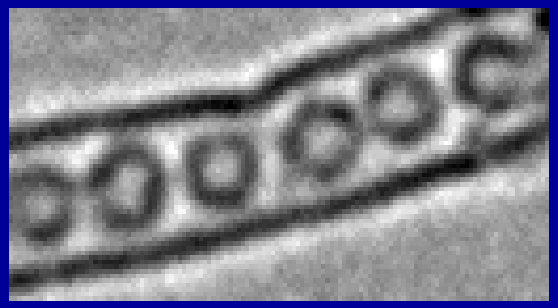


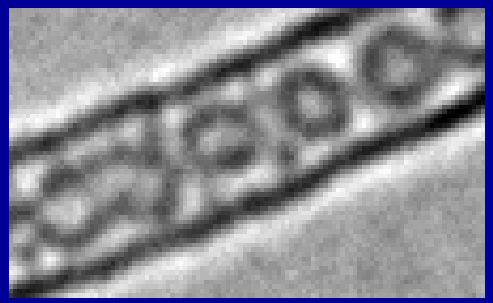


Chemical analysis of single Gd atoms inside peapods

Intercalation-site of alkali metal in K-doped peapod







Peking University
(prof. Gu and Shi)

HR-TEM being updated

Resolving C-C distance (0.14 nm) with an aberration corrected TEM at 120 kV (unpublished)

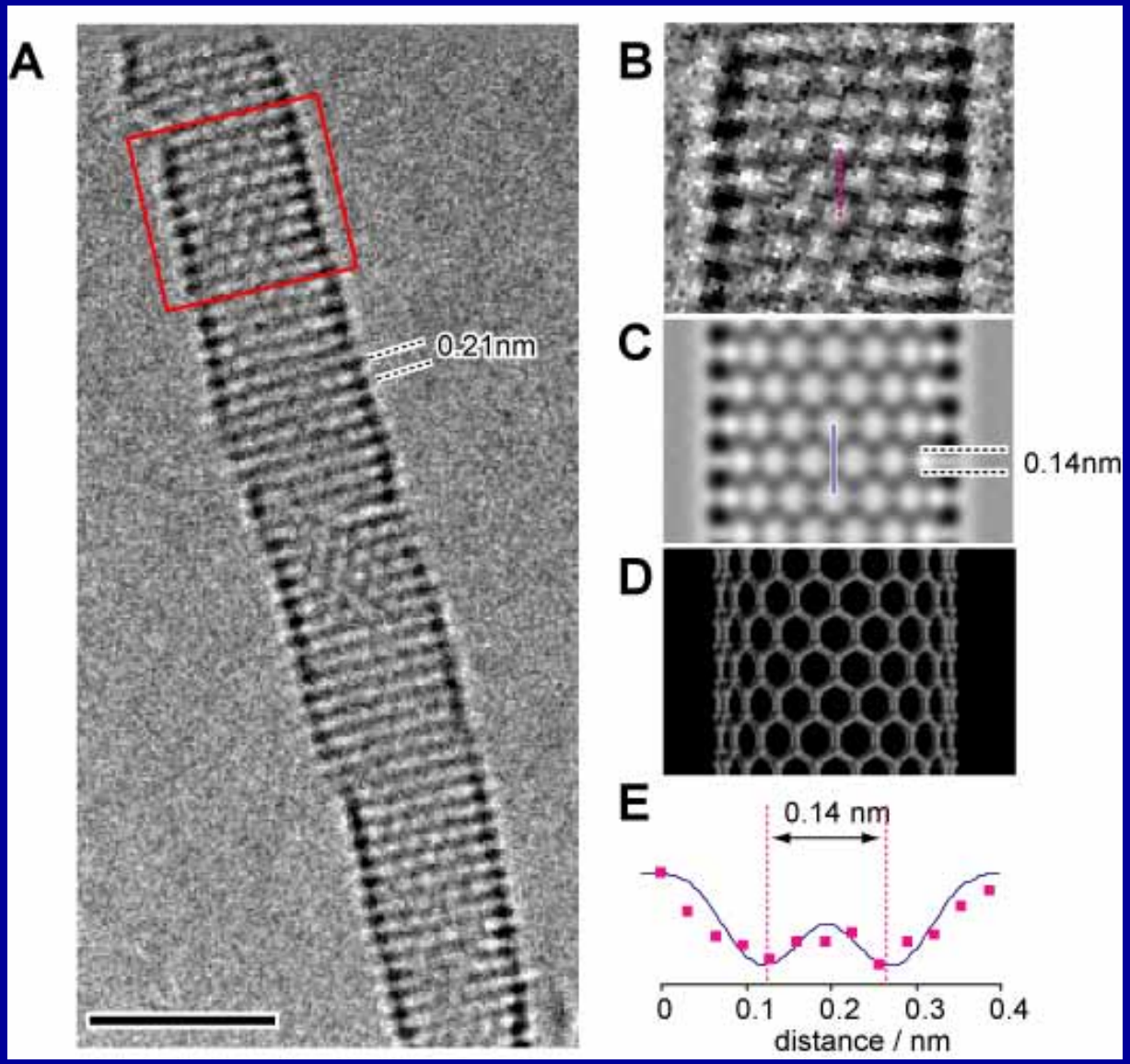
An aberration corrected HR-TEM

How can we see carbon atoms in phase contrast?

- C-C bond rotations (the StoneWales transformation)
- Alkyl chains (-C-C-C-C-)
- Conjugated carbon chains (-C=C-C=C-)
- Carbon dimers (C-C)
- Individual methyl groups ($-CH_3$)

Known problems
– irradiation damage of electron (knock-on, ionization,,,,)

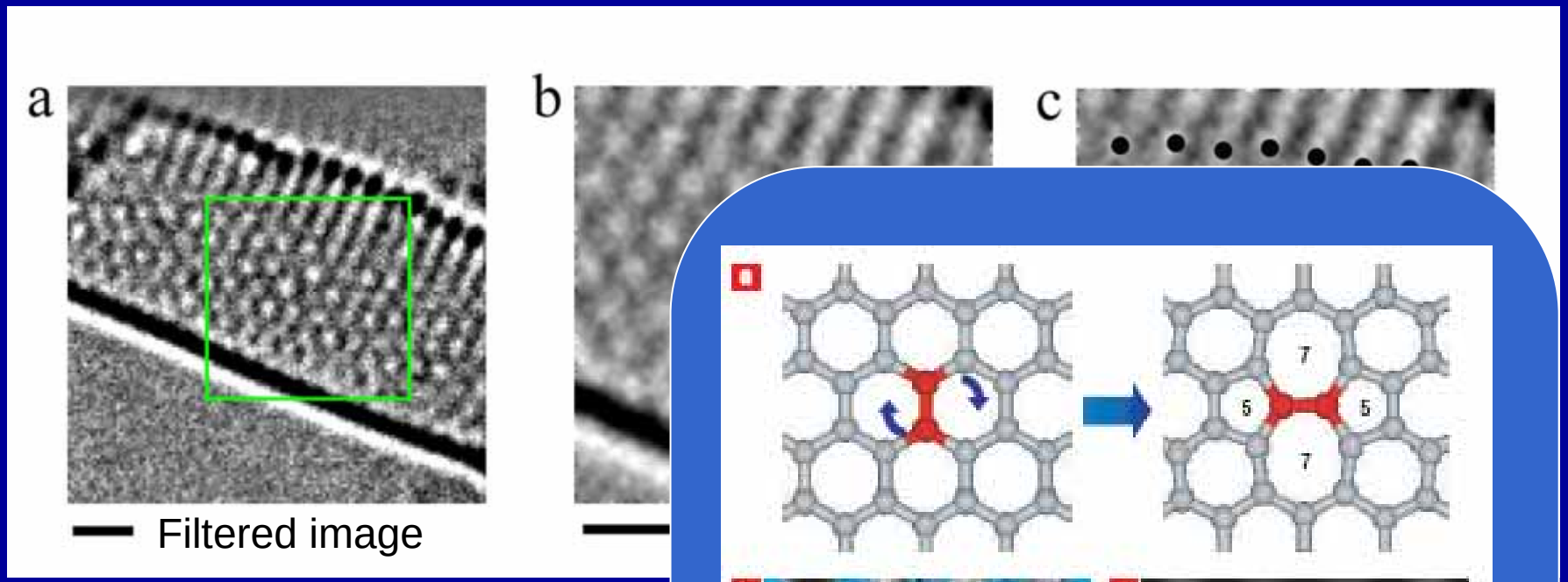
SWNT (18, 0)
HR-TEM with Cs corrector

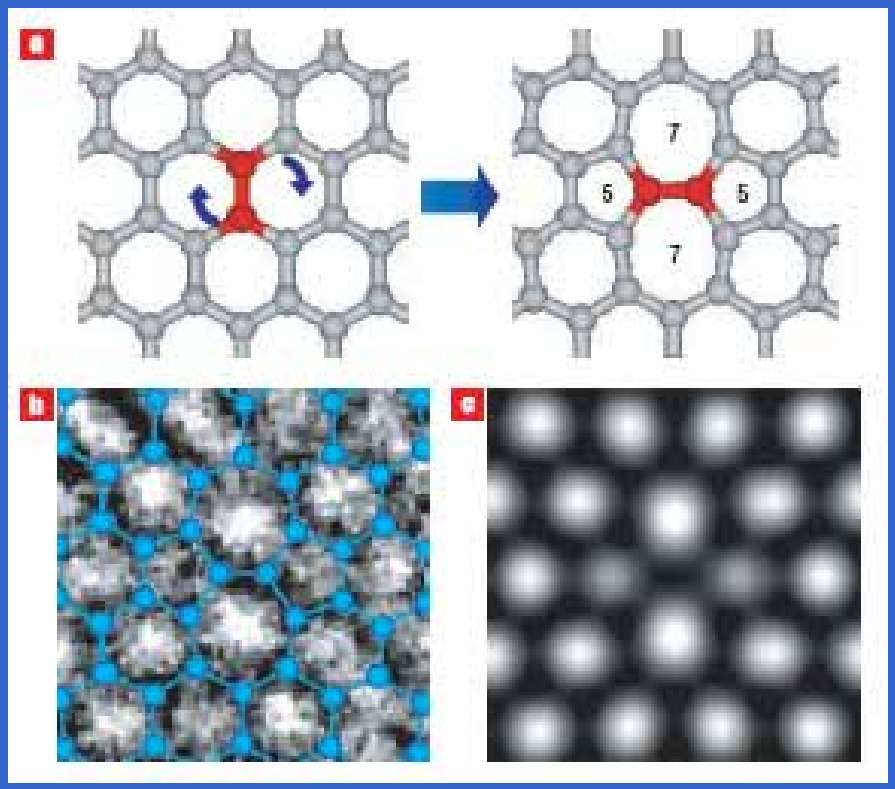


C-C bond (0.14nm) resolution

M. Koshino

Identification of atomic defects

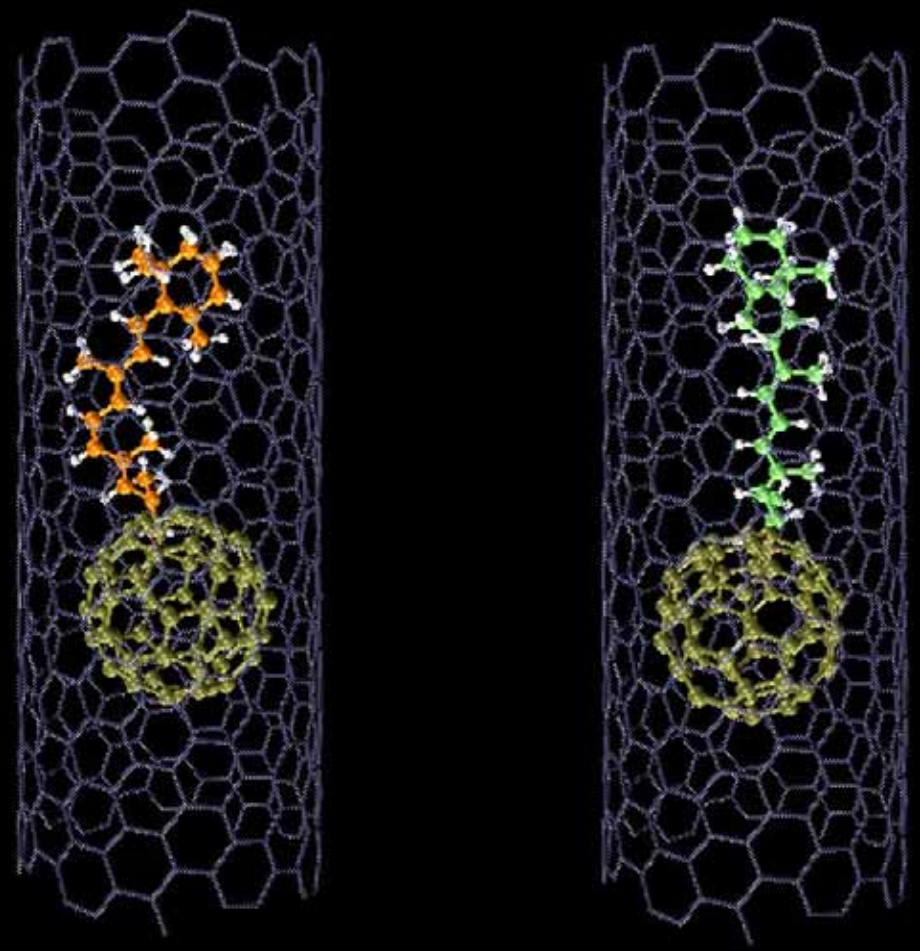




5-7-7-5 defect
(the Stone-Wales transformation)
(relaxed by using the PWC functional)

Nature Nanotech (2007)

Retinal-C_{60} (all-trans and 11-cis)

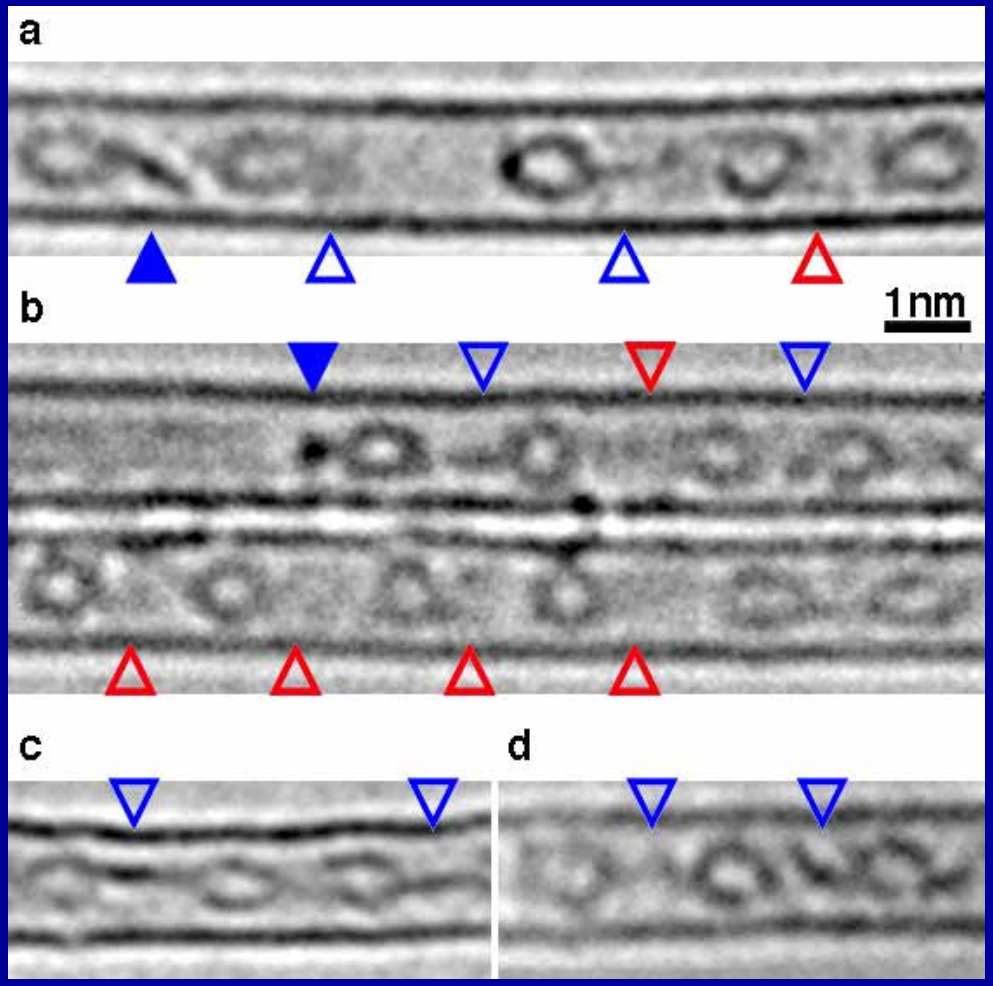


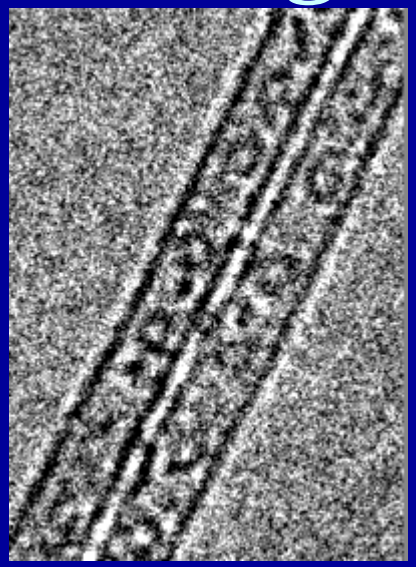
Specimen:
Kataura and Yanagi

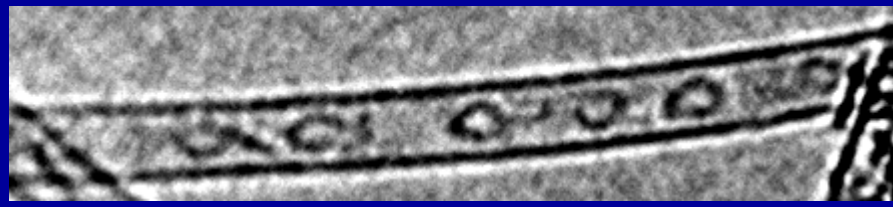
Encapsulation:
Reflux in chroloform

C_{60} acts as a tugboat to put the molecules inside.

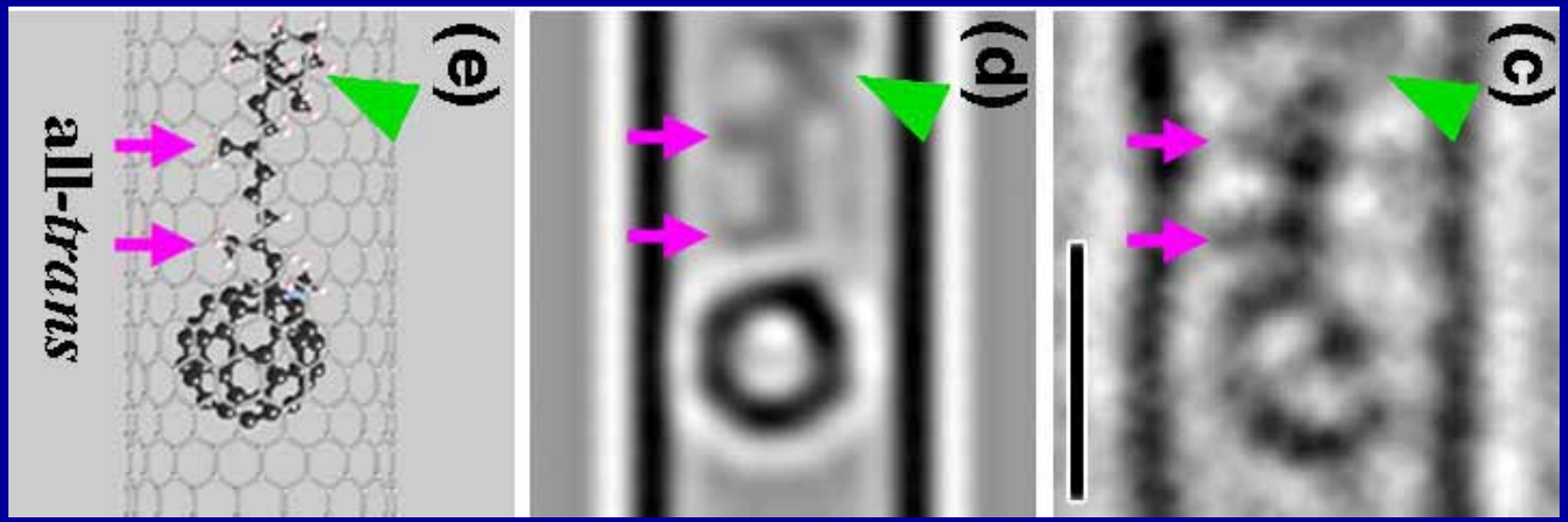
Time-averaged HR-TEM images





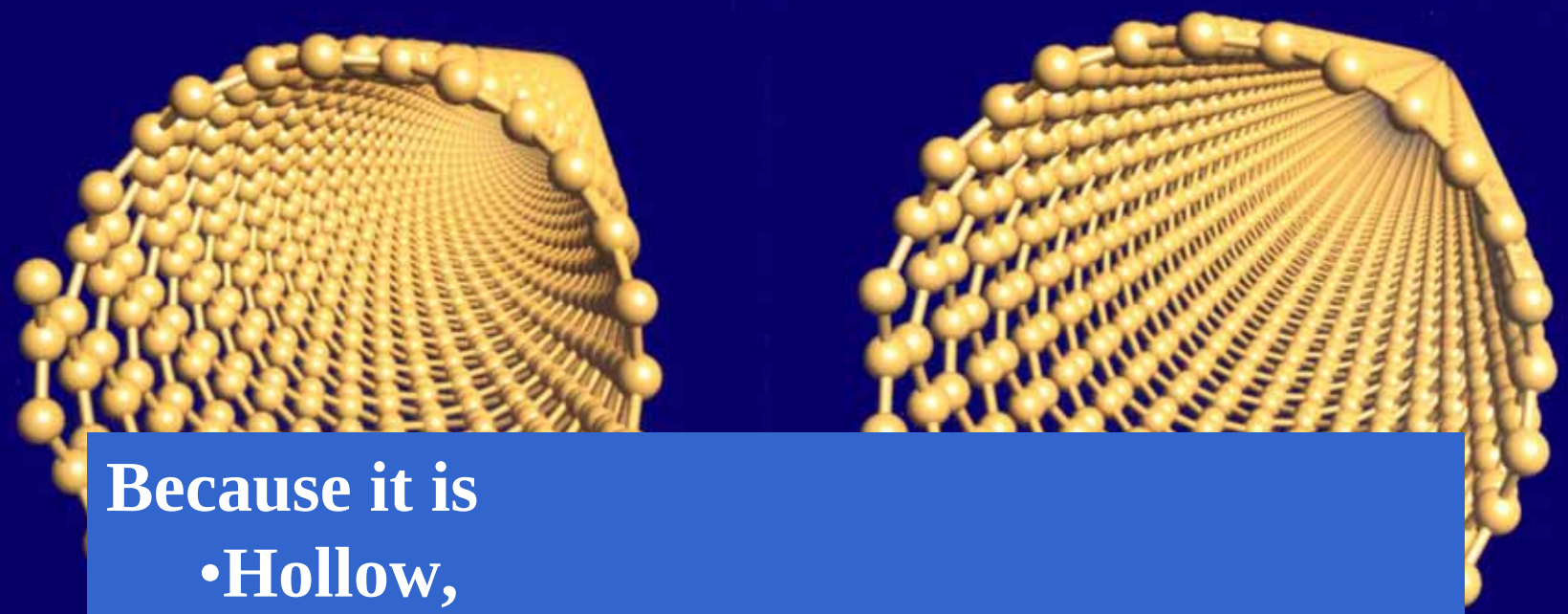


HR-TEM of all-trans retinal with fine structures



Even a cyclohexene and methyl groups can be visualized.

The carbon nanotube is ideal for a nanoscopic specimen cell!



Because it is

- **Hollow,**
- **Made of the light element,**
- **Extremely thin (single-layer),**
- **And atomically flat,**

Then provides the lowest background noise.

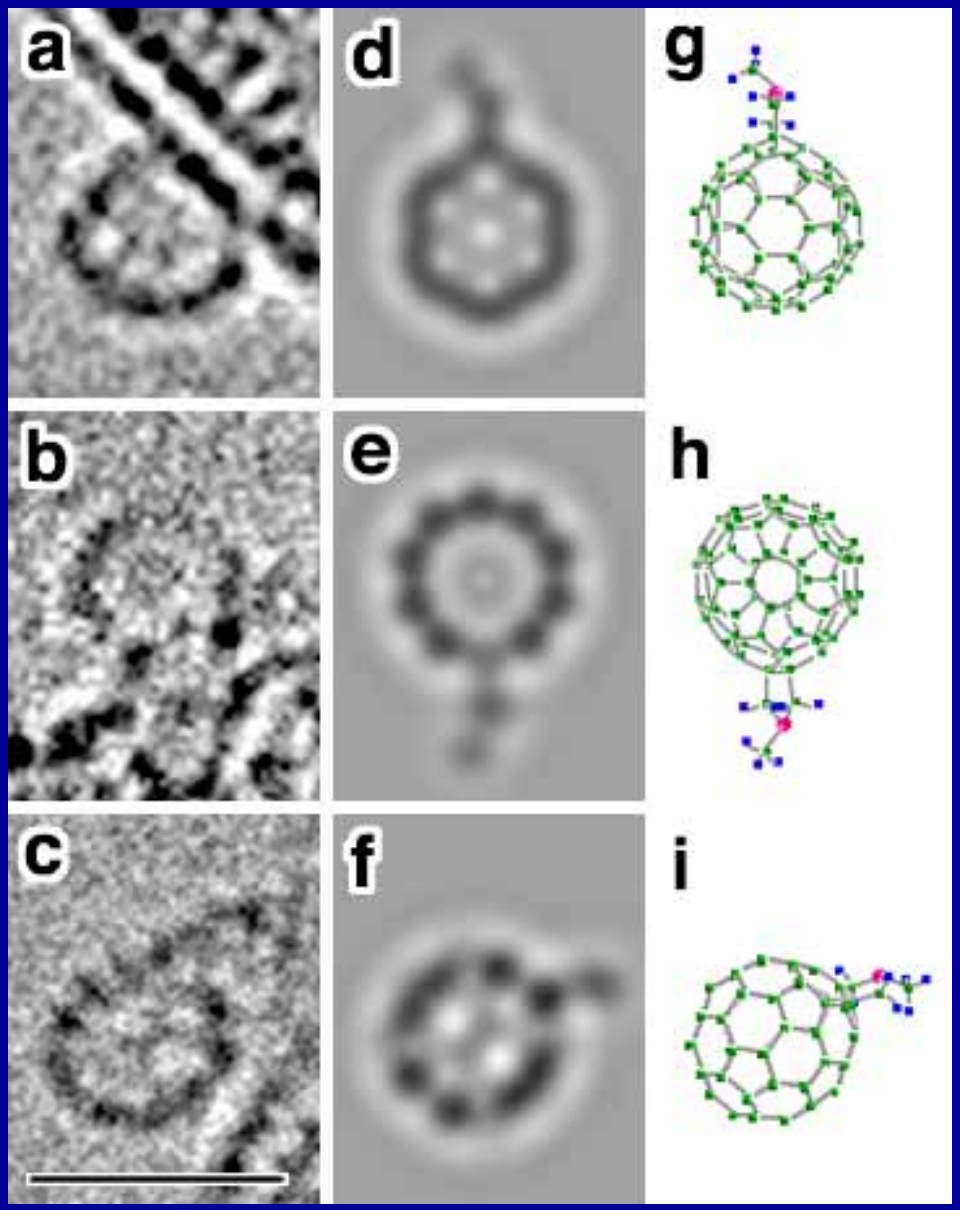
Individual molecular imaging of fullerenes by a HR-TEM with a Cs corrector

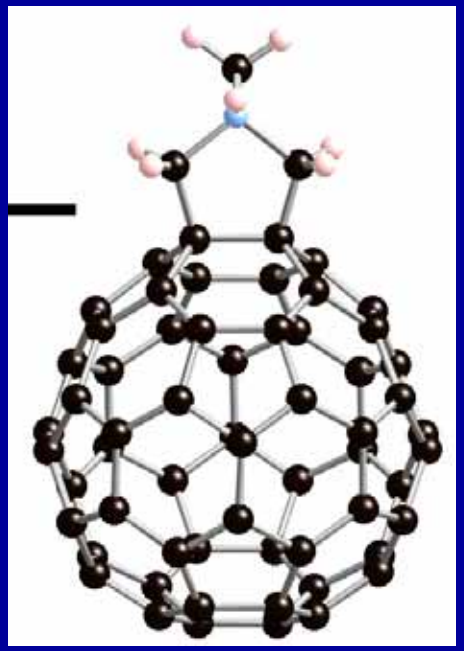
Liu et al., JACS (2007)

Wakabayashi et al., (unpublished work)

Sato et al., (unpublished work)

Imaging individual molecular structures





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