Carbon Nanocapsules

blocking materials inside carbon nanotubes

Gerard Tobias

Belén Ballesteros, Lidong Shao, Malcolm L. H. Green

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UNIVERSITY OF OXFORD

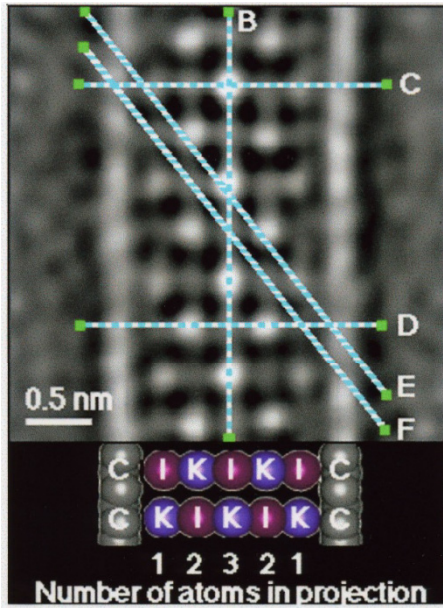
Outline

- ✓ *Introduction*
- ✓ *Purification and opening of SWNTs*
- ✓ *Formation of carbon nanocapsules*
  - ✓ *Closing the ends of carbon nanotubes*
  - ✓ *Use of fullerenes as "corks"*
- ✓ *Summary*

Encapsulation of materials inside SWNTs

Growth of 1D crystals

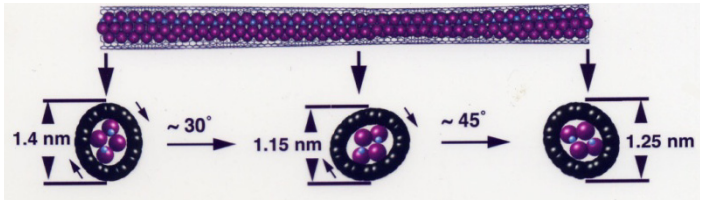
KI@SWNT



Change of interatomic distances

Science 289, 1324 (2000)

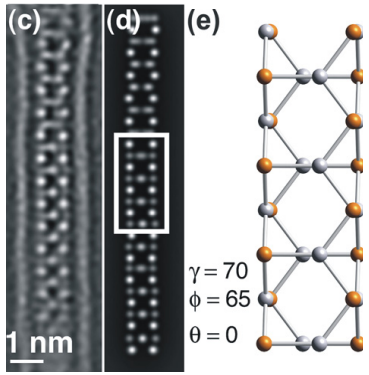
CoI_2@SWNT



Simultaneous rotation of crystal & SWNT

Nature Materials 2, 788 (2003)

HgTe@SWNT



New coordination geometries

Modified electronic structure

Band gap (DFT)

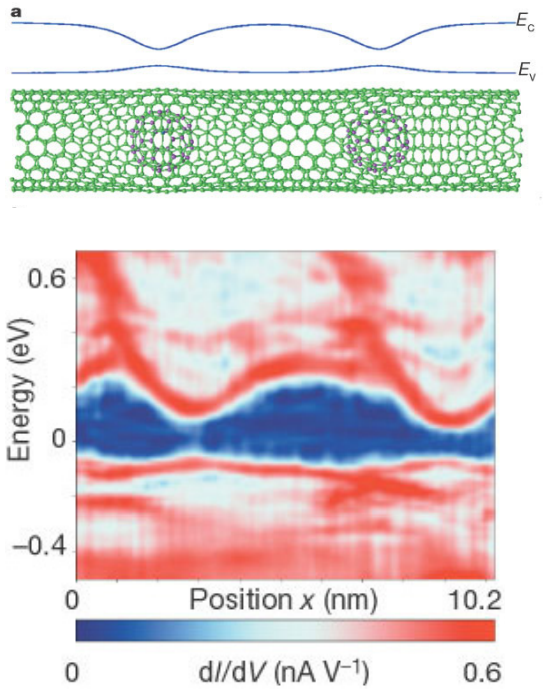
1D HgTe = 1.20 eV

PRL 96, 215501 (2006)

Encapsulation of materials inside SWNTs

Modulation of the electronic structure

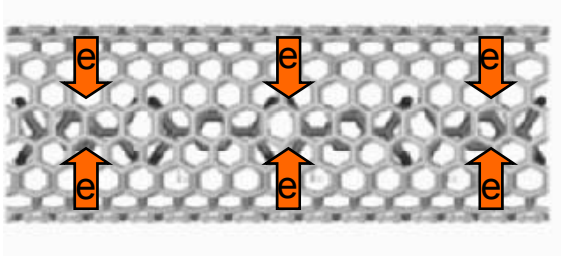
SWNTs filled with $Gd@C_{82}$



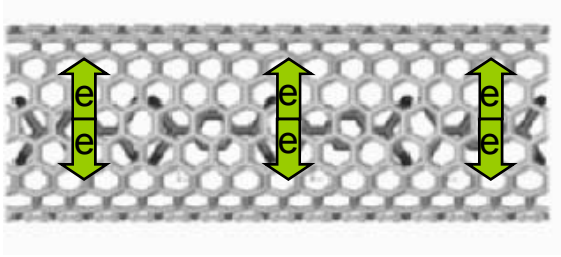
Nature 415, 1005 (2002)

Doping of CNTs by filling:

p-doping (I_x, TCNQ)



n-doping (Cs, TDAE)

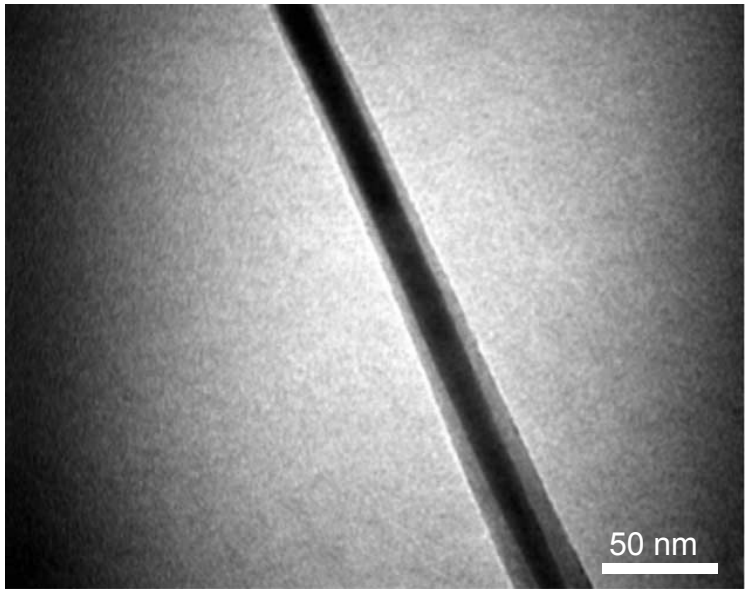


Nat. Mater. 2, 683 (2003)
Chem. Commun. 3429 (2008)

Encapsulation of materials inside CNTs

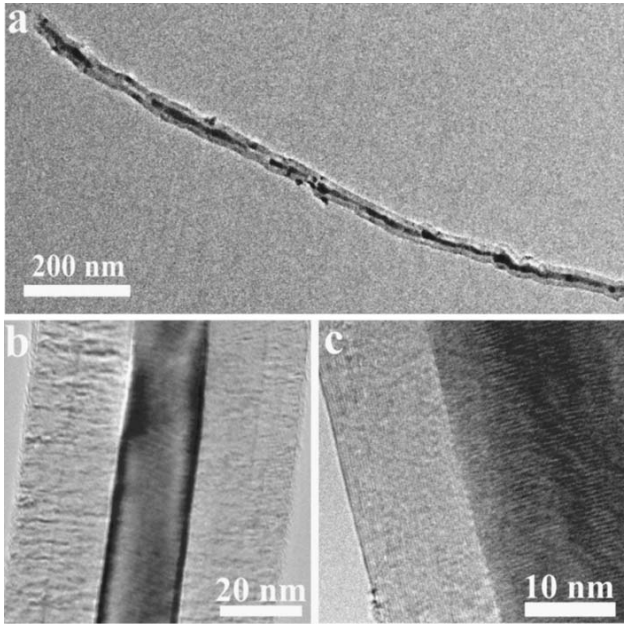
Encapsulation of magnetic materials - High density data storage

Ni@MWNTs



Thin Solid Films 469, 127 (2004)

Fe@MWNTs



J. Appl Phys. 103, 034302 (2008)

Purification and opening of SWNTs

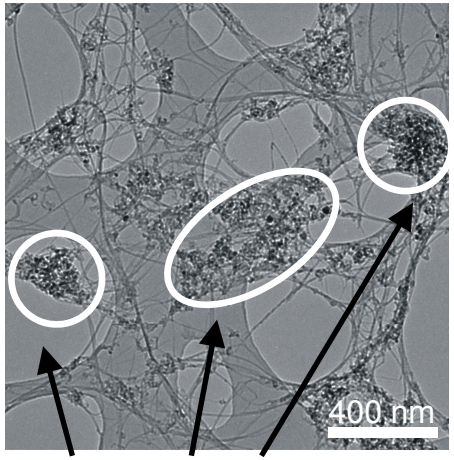
Impurities in CNTs

- Amorphous carbon
- Graphitic particles
- Metal particles (catalyst)

Most purification strategies damage CNT structure

Steam treatment at 900 °C, 4h (CVD SWNTs – Elicarb)

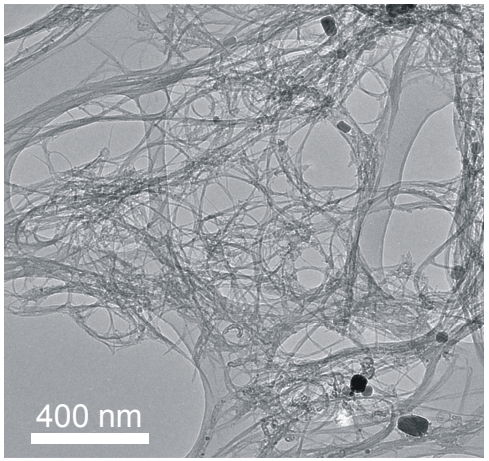
As-made SWNTs



Amorphous carbon and graphitic shells

steam
H_2O

Purified SWNTs



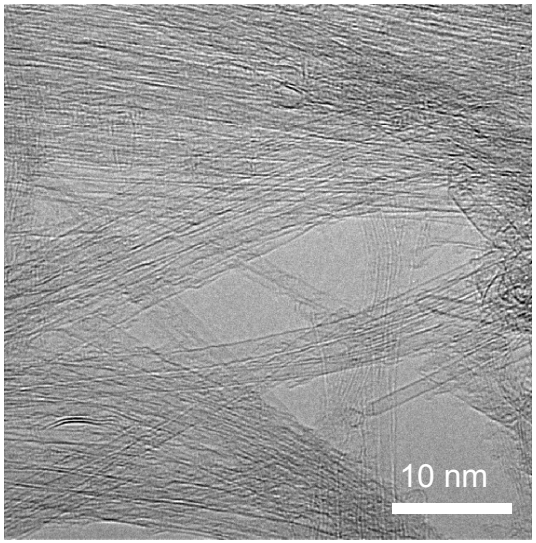
No amorphous carbon
Metal particles free of graphitic coating (HCl)

J. Phys. Chem. B 110, 22318 (2006)

Small 4, 1501 (2008)

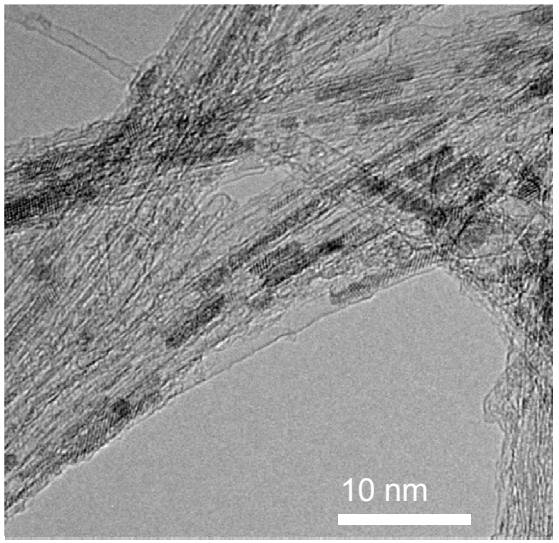
Open-ended SWNTs

Steam treated SWNTs



Solution filling
Uran. Ac.

Filled SWNTs



STEAM

- Removes amorphous carbon
- Removes graphitic shells coating metal particles (dis. in HCl)
- Opens the ends of CNTs
- Long treatments result in shorter CNTs
- The CNT tubular structure is preserved (even after long treatments)
- No functional groups are detected by XPS and IR spectroscopy

J. Phys. Chem. B 110, 22318 (2006)

Small 4, 1501 (2008)

Formation of carbon nanocapsules

Filling of CNTs
- Solution filling
- Vapour filling
- Melting filling

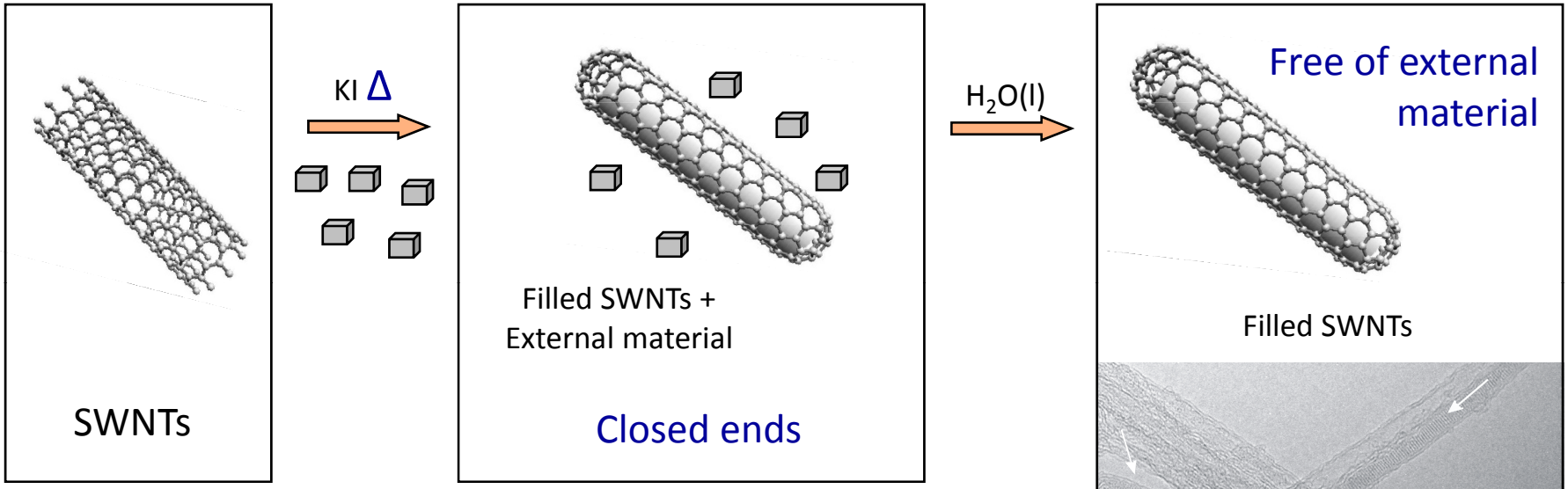
Large amount of UNWANTED external material

Ends of SWNTs need to be closed – sealed

to allow purification of carbon nanocapsules

Closing the ends of SWNTs

MELTING FILLING



Limitations of this approach

- Thermal stability - not useful for organic molecules-
- Low reactivity with carbon
- Surface tension < 170 mN/m *(Adv. Mater. 10, 1472, 1998)*

Allows a quantitative assessment of the encapsulated material

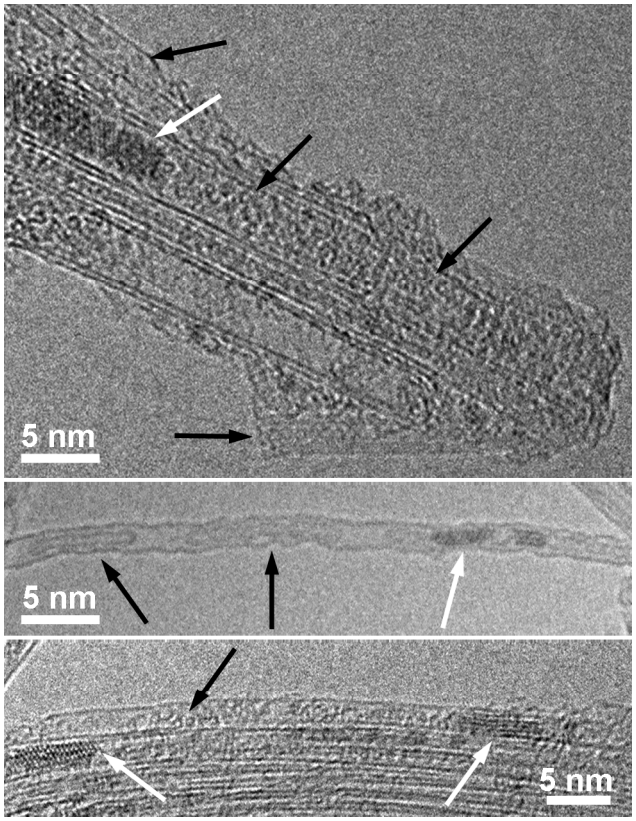
Carbon 44, 2855 (2006)

J. Phys. Chem. C 113, 2653 (2009)

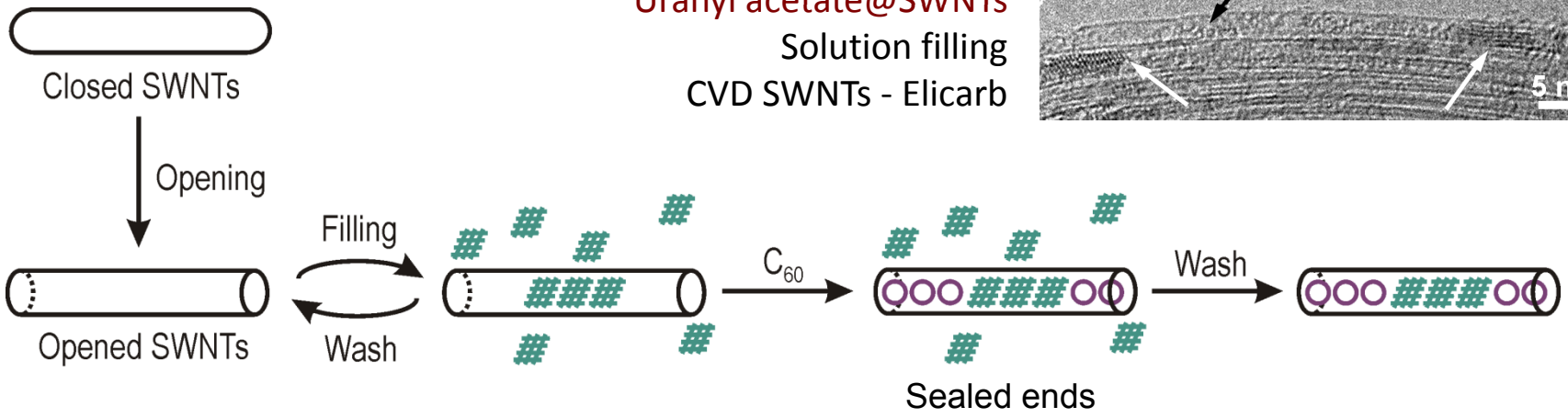
Use of fullerenes as "corks"

SOLUTION FILLING (low T)

1) Stir open-ended SWNTs
   in a solution of desired compound
2) Block the ends with fullerenes
3) Removal of external material



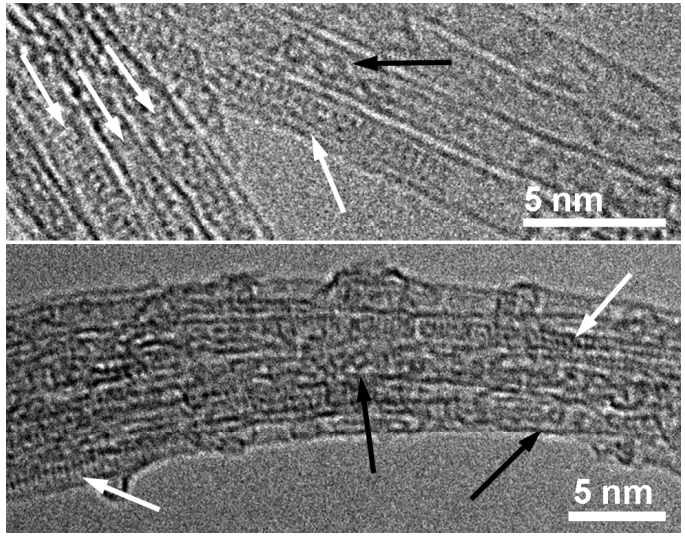
Uranyl acetate@SWNTs
Solution filling
CVD SWNTs - Elicarb



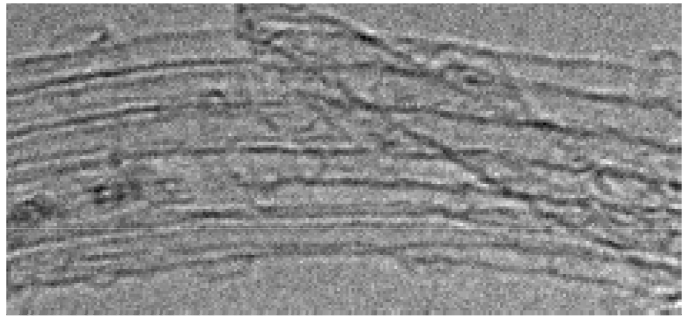
Chem. Commun. 44, 2164 (2008)

Use of fullerenes as "corks"

KI@SWNTs

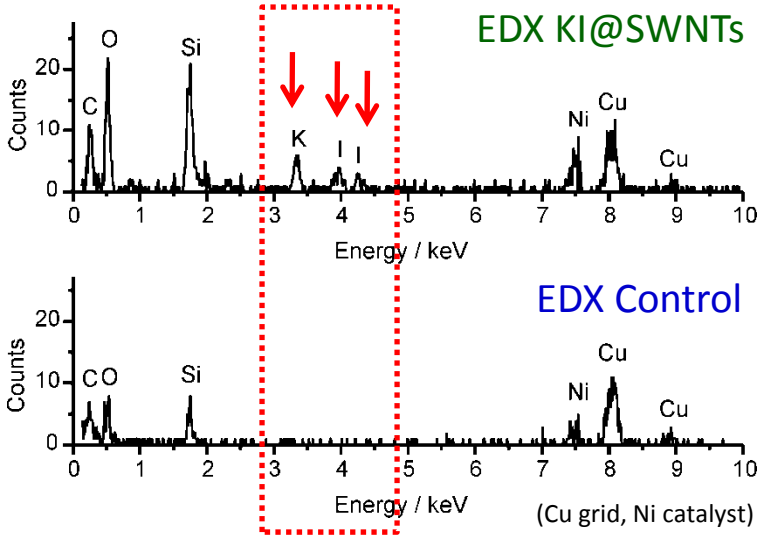


Control



Sample preparation:

Melting filling + Opening
Arc SWNTs



Chem. Commun. 44, 2164 (2008)

Summary

- ✓ *Steam treatment allows the purification and opening of carbon nanotubes without altering their tubular structure.*
- ✓ *Carbon nanocapsules of filled SWNTs with closed ends can be obtained in one-step by melting filling at high temperature.*
- ✓ *Fullerenes can be used as corks for the containment of soluble materials inside carbon nanotubes.*

Acknowledgements

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