SIZE EFFECTS & QUANTUM MECHANICS GOVERNED PHENOMENA IN NANO-SYSTEMS

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United Nations Educational, Scientific and Cultural Organization

UNESCO-UNISA Africa Chair in Nanosciences/Nanotechnology (South Africa)

ANDERSON LOCALIZATION, CONFINEMENT, MOTT PHASE TRANSITION, & QUATUM OPTICS IN NANO-SCALED SYSTEMS

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Department of Science and Technology

National Research Foundation

UNISA university of south africa

NRF National Research Foundation | iThemba LABS Laboratory for Accelerator Based Sciences

United Nations Educational, Scientific and Cultural Organization

International Atomic Energy Agency

The Abdus Salam International Centre for Theoretical Physics

NANOAFNET NANOSciences NETWork

ANSOLE

alc african laser centre

LAM African Laser Atomic Molecular & Optical Sciences Network

AFRICA MRS

AfPS

AFRICAN UNION

PRESENTER BIO

- PhD in Wave Matter Neutron Optics 1993
- Joint staff iThembaLABS-NRF & UNISA
- UNESCO UNISA ITLABS-NRF Africa Chair in Nanosciences & Nanotech
- Research interest: Nanoscale
- Fellow of the African Academy of Sciences
- Fellow of the Royal Society of Chemistry-London
- Fellow of the National Academy of Sciences of India
- Fellow of the New York Academy of Sciences
- Fellow of the Islamic Academy of Sciences
- Fellow of the European Academy of Sciences
- Fellow of the American Association for Advancement of Science
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OUTLINE

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2-HISTORICAL BACKGROUND: FROM FARADAY TO FEYNMAN

3-NANO-MERCURY:RELATIVISTIC & DIRAC CORRECTIONS

4-C.-NANOTUBES: LIGHT ANDERSON LOCALIZATION

5-ZnO NANOPLATES:SURFACE TENSION TUNABILITY

6-NANO-SCALED SYSTEMS & FORESIGHT: AI & MULTI-DISCIPLINARITY

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MULTISKILLED Human Capital DEVELOPMENT-

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MULTISKILLED Human Capital DEVELOPMENT-

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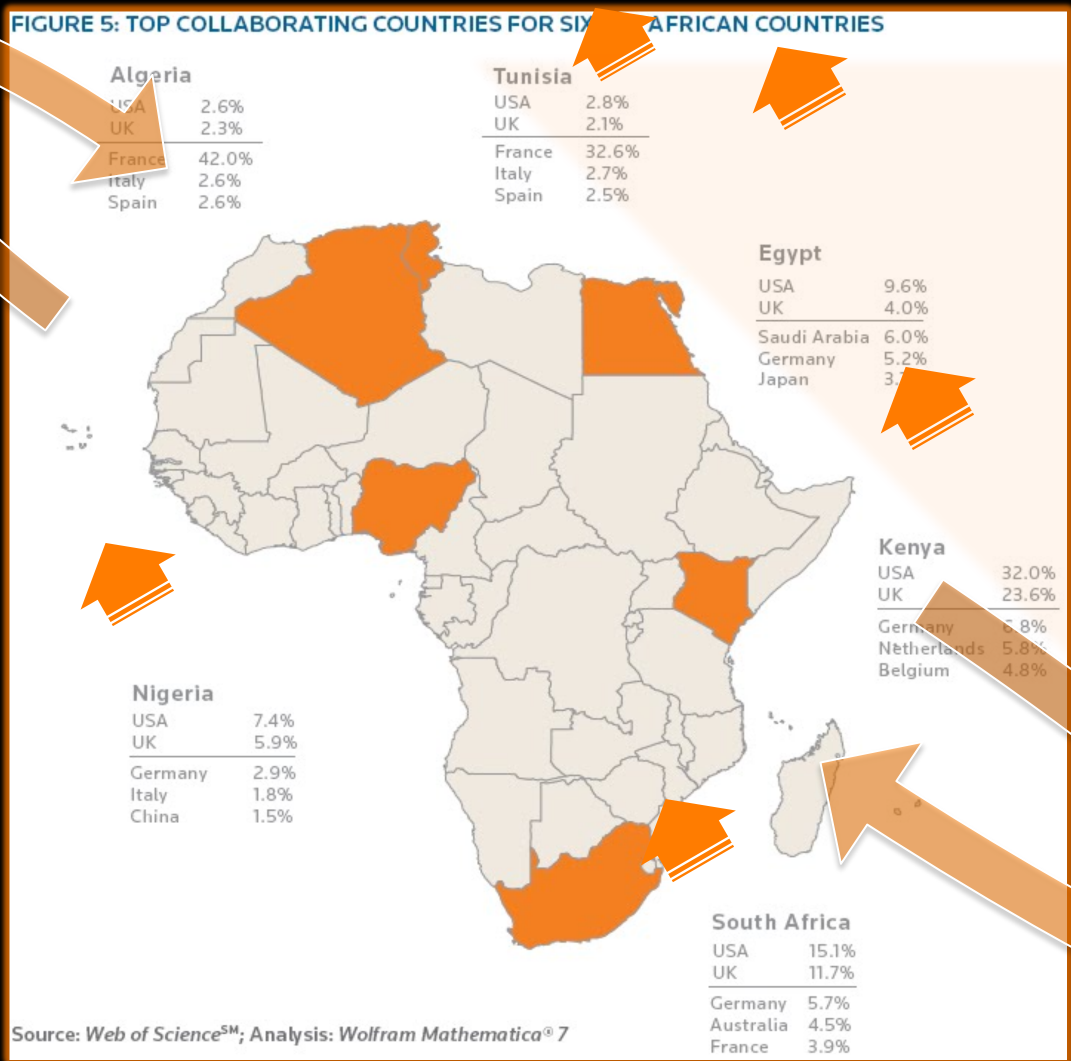

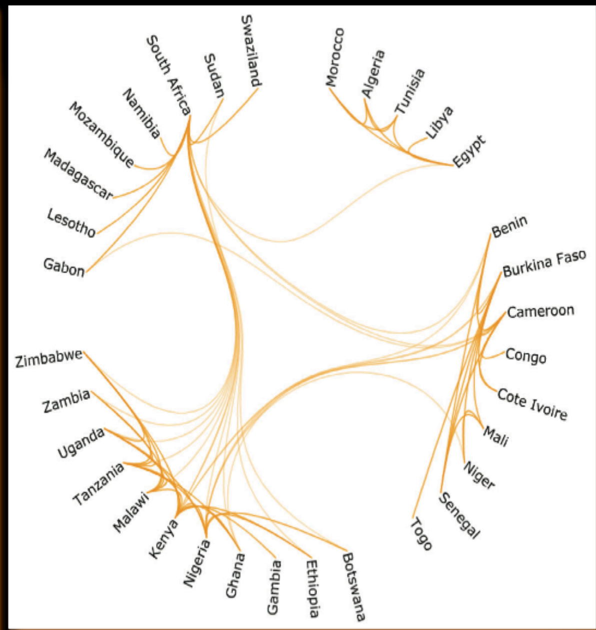

Source: OECD, Nature Publishing, World Economic Forum 2012

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Contents lists available at ScienceDirect

Applied Surface Science

journal homepage: www.elsevier.com/locate/apsusc

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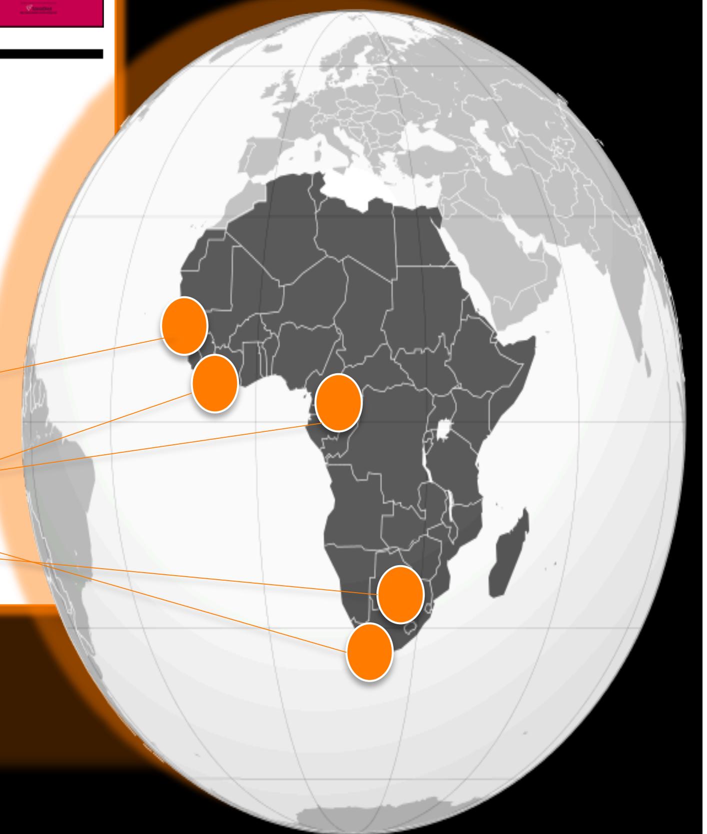
[f] Department of Physique University of Yaoundé 1, Cameroon
[g] Centre for Energy Research and Development, Obafemi Awolowo University, Ile-Ife, Osun State, Nigeria



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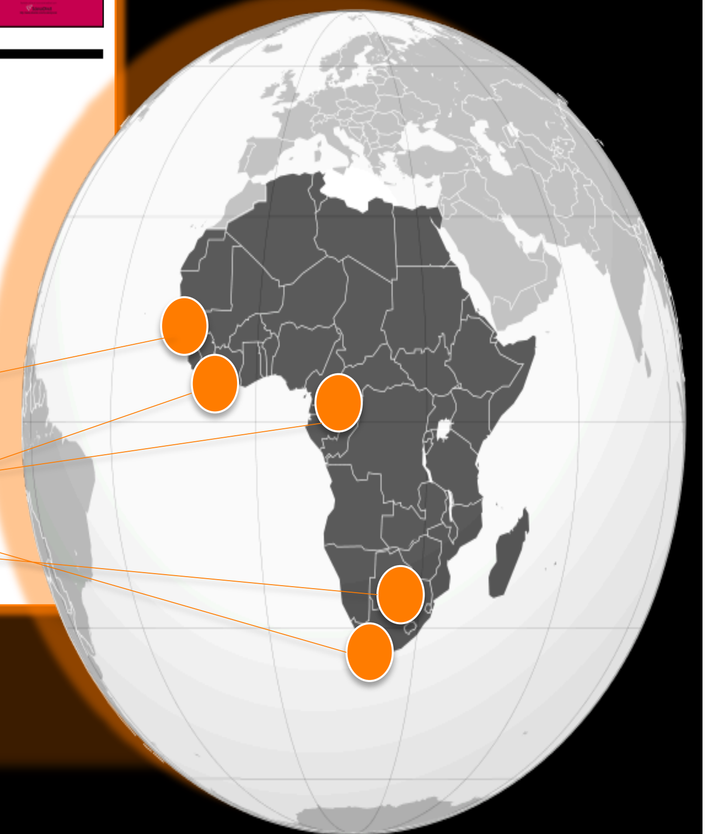

U2ACN2: UNESCO UNISA ITLABS/NRF AFRICA CHAIR IN NANOSCIENCES & NANOTECHNOLOGY

RESEARCH FOCUS:

- Nanomaterials for Energy
- Nanophotonics,
- Nanomaterials by green Processing,
- Nanomaterials & biomimics,
- Nanomaterials & Radiations:

I-Nanostructures for neutrons trapping & neutron life time
II-H^+ induced magnetism in Carbon based nanosystems,
III-H^+induced Superconductivity in WO_{3-d} bronzes,
IV-Nano-suspensions by γ-radiolysis,
V-IBA Radiations hardness of nanomaterials.

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NANO-1:
RELATIVISTIC CONTRACTION & DIRAC CORRECTION

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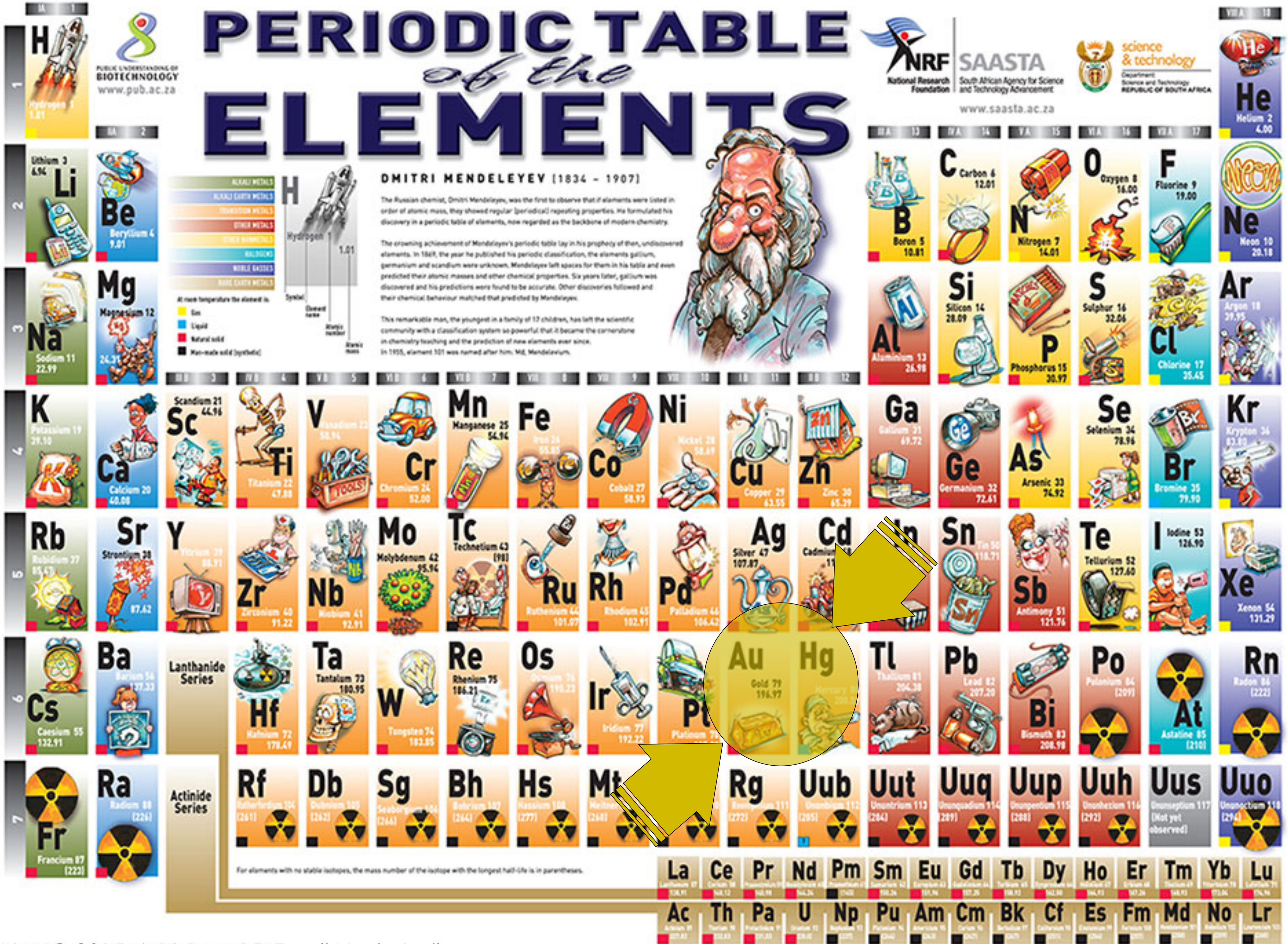

PERIODIC TABLE
of the
ELEMENTS
DMITRI MENDELEYEV (1834 – 1907)
Lanthanide Series
Actinide Series
NRF
SAASTA
science & technology
www.saasta.ac.za
www.pub.ac.za

RELATIVISTIC CONTR. & DIRAC CORREC.

–Surface Tension: Hg

Hg swimming pool

Archimedes

$\sim \rho g V$

Mercury Telescope Spins Up

Pending solid science from the new Large Zenith Telescope, a group of scientists hopes to build an extremely large—and extremely cheap—array of liquid mercury telescopes.

Liquid mirrors have one single advantage. Only one. It's cost," says Ermanno Borra of Laval University in Quebec, Canada. In the early 1980s, Borra resurrected the idea of liquid mirror telescopes, first put forth in 1850 by the Italian astronomer Ernesto Capocci. The disadvantage is that they can't be tilted, he says. "You are stuck with the strip of sky above you. But it's not as bad as it sounds."

Liquid mirror telescopes are suited to surveying classes of objects and to studying supernovae and other variable phenomena. "Look at Paul [Hickson]," says Borra. "He has a 6-meter telescope to do cosmology. With a conventional glass mirror, you can cover the whole sky, but you have to share with a lot of people. Cost, cost, cost. That's what it's all about."

Hickson, an astronomer at the University of British Columbia, Canada, spearheaded the Large Zenith Telescope, the newest and biggest liquid mirror telescope. It is located about 60 kilometers east of Vancouver and partners come from Laval University, the Institut d'Astrophysique de Paris, SUNY Stony Brook, and Columbia University. The LZT cost about $500 000, says Hickson. "If you include the parts we borrowed, it would be about $1 million." That's more than an order of magnitude less than what a glass mirror telescope of similar size would cost.

Liquid assets

The cost difference lies largely in the ease of spinning a liquid into a smooth parabola com-

Atomic roughness

$\sigma \sim 0.5$Å

RELATIVISTIC CONTR. & DIRAC CORREC. –Surface Tension

Ground State Configuration

- **Au[Kr] $5d^{10}6s^1$,**
- **Hg[Kr] $5d^{10}6s^2$, Noble gas behaviour**
- **Th[Kr] $6s^2 6p^1$,**

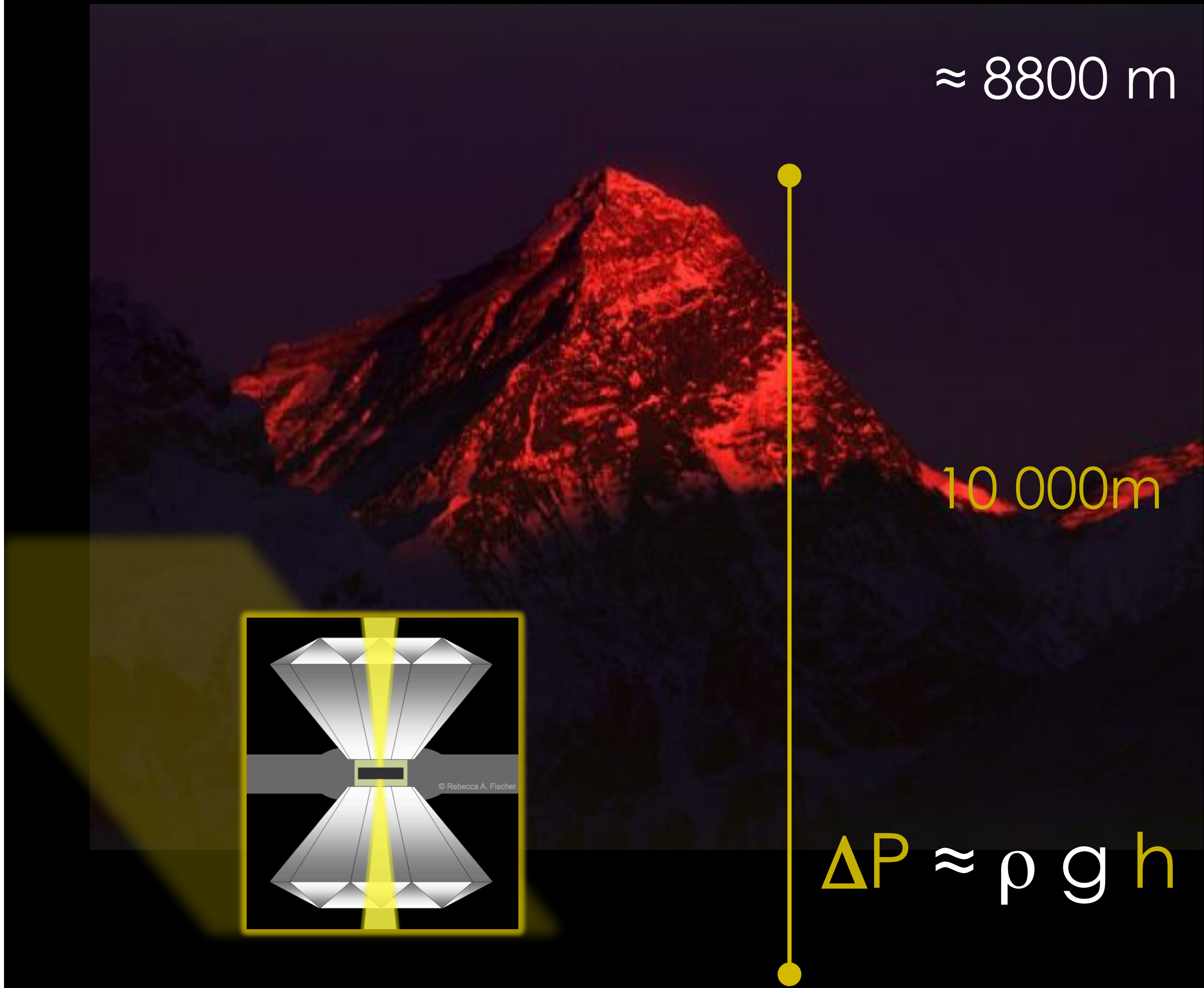
- **Relativistic contraction & "S" orthogonality:**

- **$m_e = m_0/\sqrt{(1-v/c)}$**
- **$r_0 = 4\, e_0\, h^2 /\, p\, e^2\, m_e$**

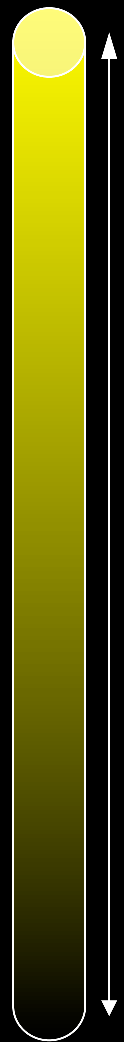
- **Relativistic contraction of "S" Orbitals:**
"1s" shell electrons: v/c =80/137 ≈0.58:Radial shrinkage of 23%
- **Valence electrons less bounded:**

RELATIVISTIC CONTR. & DIRAC CORREC.

–Surface Tension: Hg



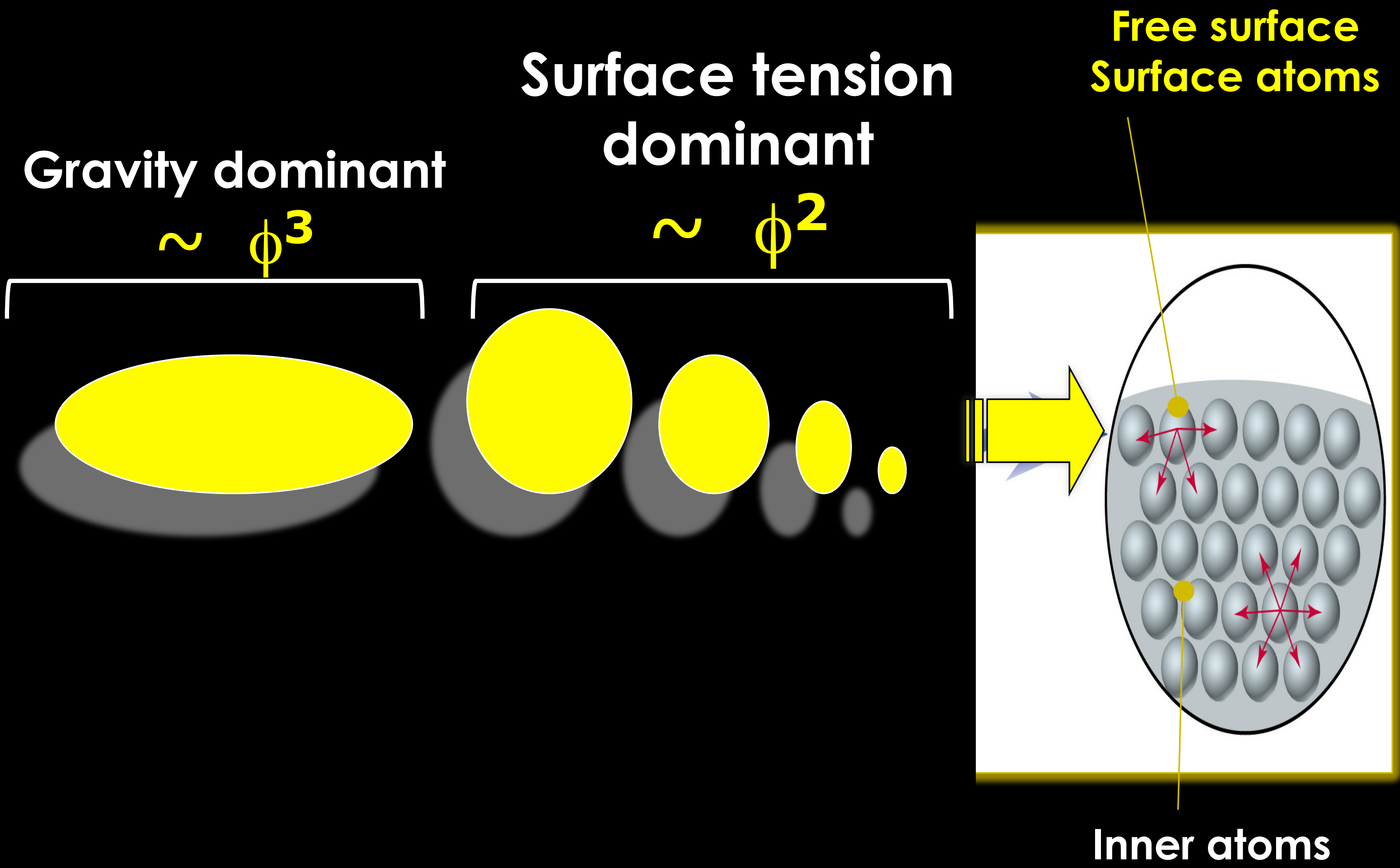
Top: Liquid



Bottom: solid

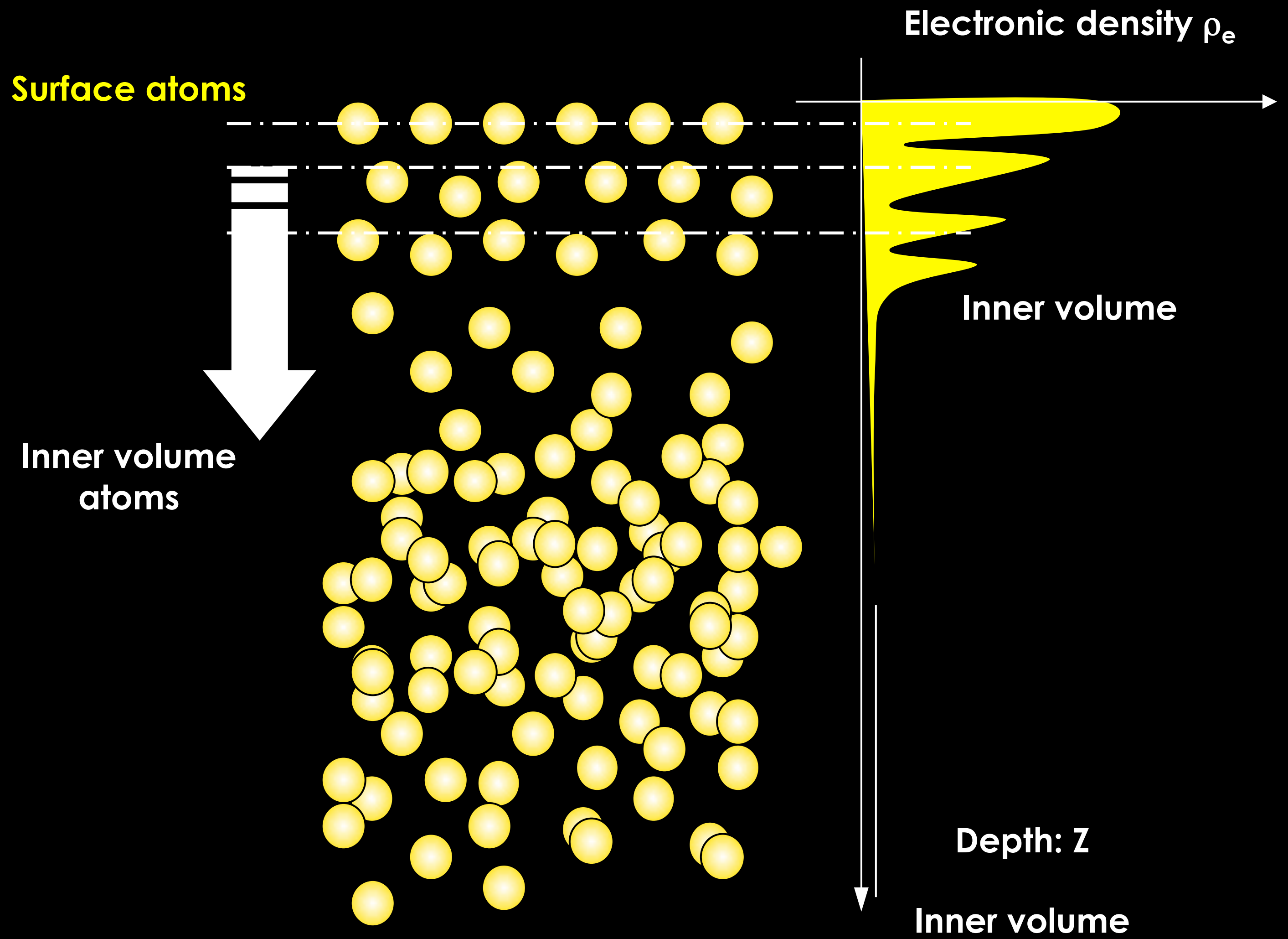
RELATIVISTIC CONTR. & DIRAC CORREC.

–Surface Tension

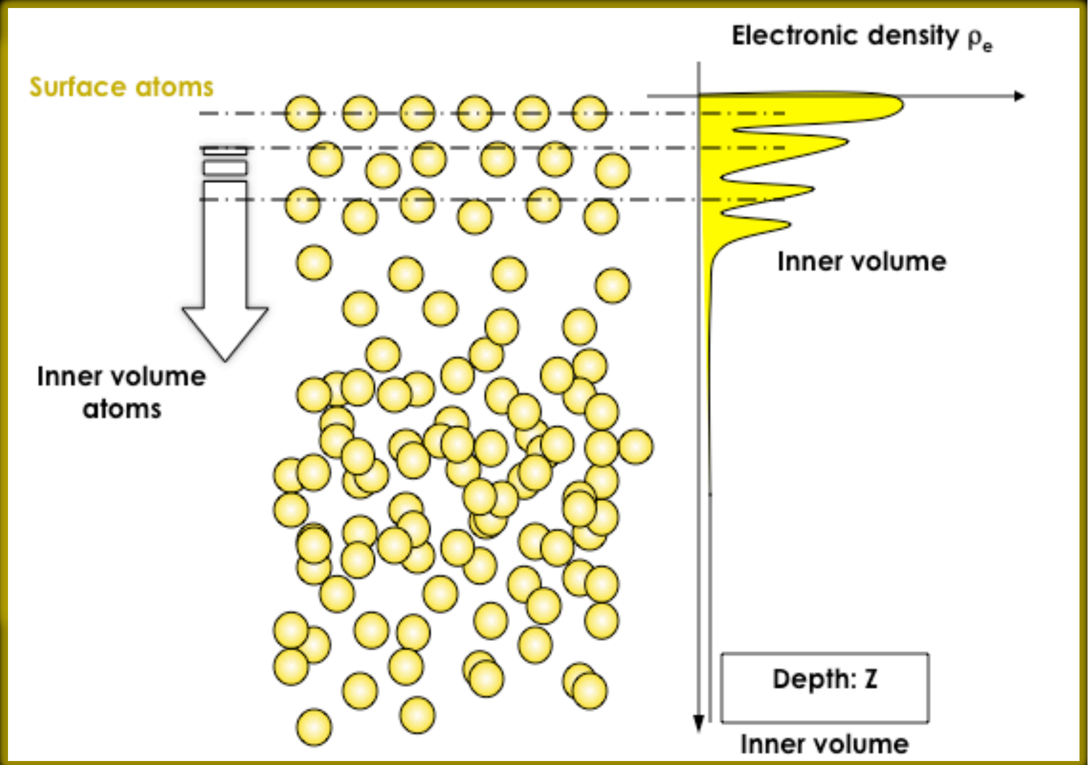


Highest Surface Tension@ 293K: $\gamma \approx 486\ 10^{-3}$ SI

NANO: LOCALIZATION & CONFINEMENT –Surface Tension



NANO: LOCALIZATION & CONFINEMENT –Surface Tension



THEORETICAL PREDICTIONS:

- Jellium Model,
- DFT Formalism,
- Non-Local Pseudo-Potential,
- Perturbation Expansion to 2nd Order in e-ion Pseudo-Potential

"Chacon-Gomez, PRB. 1992"

SURFACE ATOMIC ORDER at Hg Liquid- INTERFACE "SOLID Hg" REQUIRES EXTERNAL HIGH PRESSURE

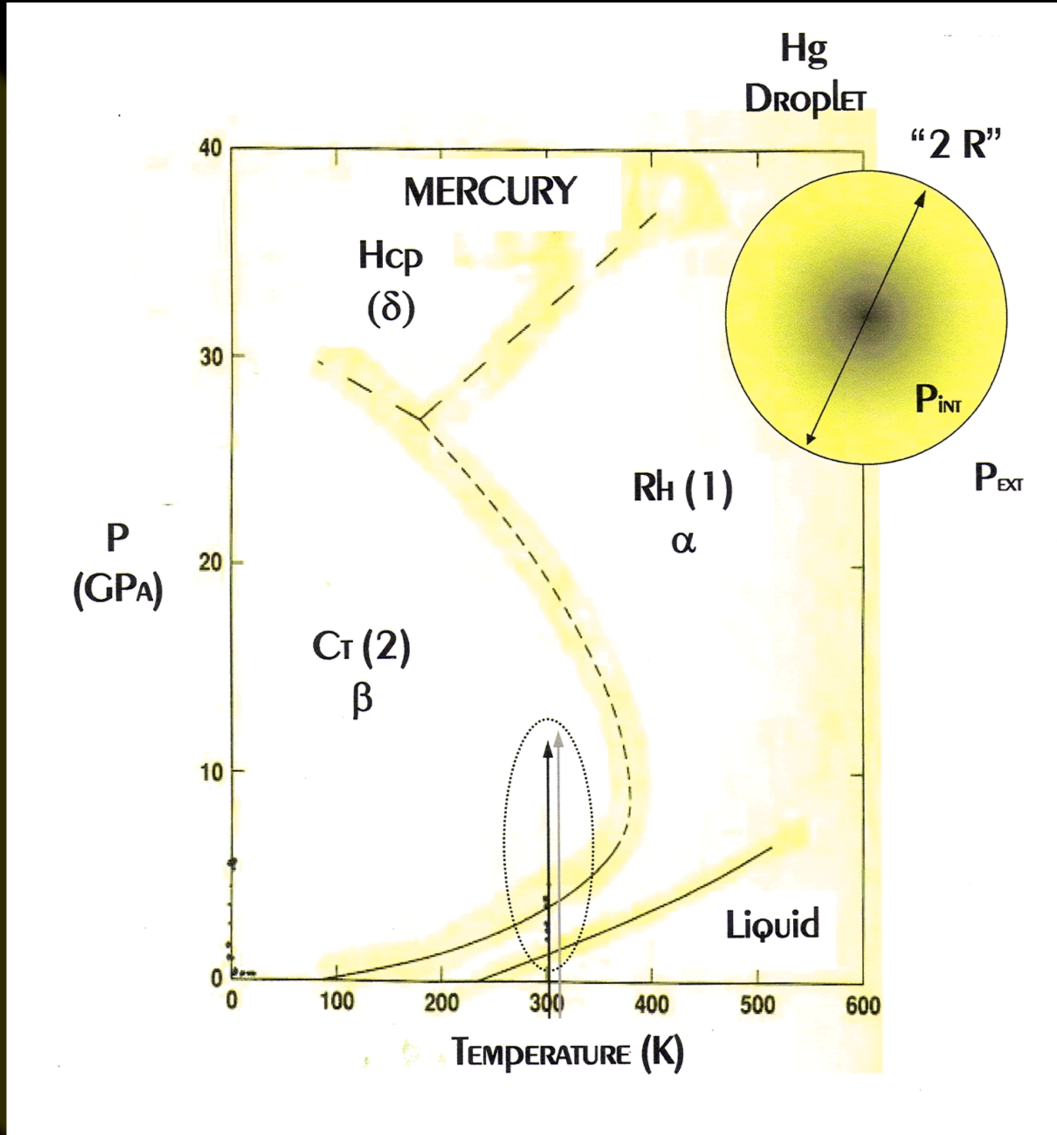
NANO: LOCALIZATION & CONFINEMENT –Surface Tension

$\Delta P \approx 8\,\gamma/\phi$,

$\gamma \approx 486\ 10^{-3}$ N/m,
0.76 GPa,

$\phi/2 \approx 1.28$ nm,

Nano-Scaled Mercury



D.A Young, in «phase Diagrams of the Elements», University of California Press, **1991**

NANO: LOCALIZATION & CONFINEMENT –Surface Tension

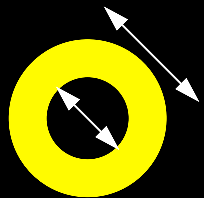
Voids

Vycor host glass
(Charnaya, 2001)

Open framework

Ultra-porous Carbon host matrix
(Kasperovich, 2003)

$Mg_3SiO_5(OH)_4$
(Chrysotile asbestos)

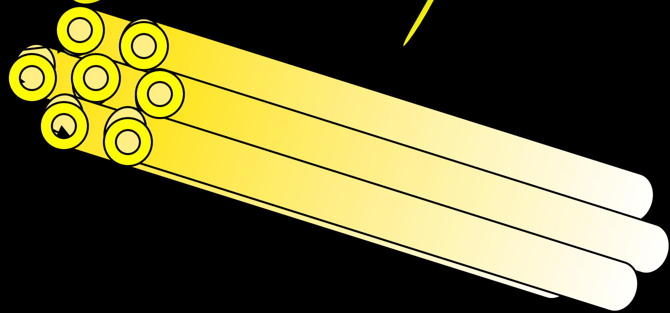


$\phi_{int} \approx 3.5$-20 nm

$\phi_{ext} \approx 30$-50 nm

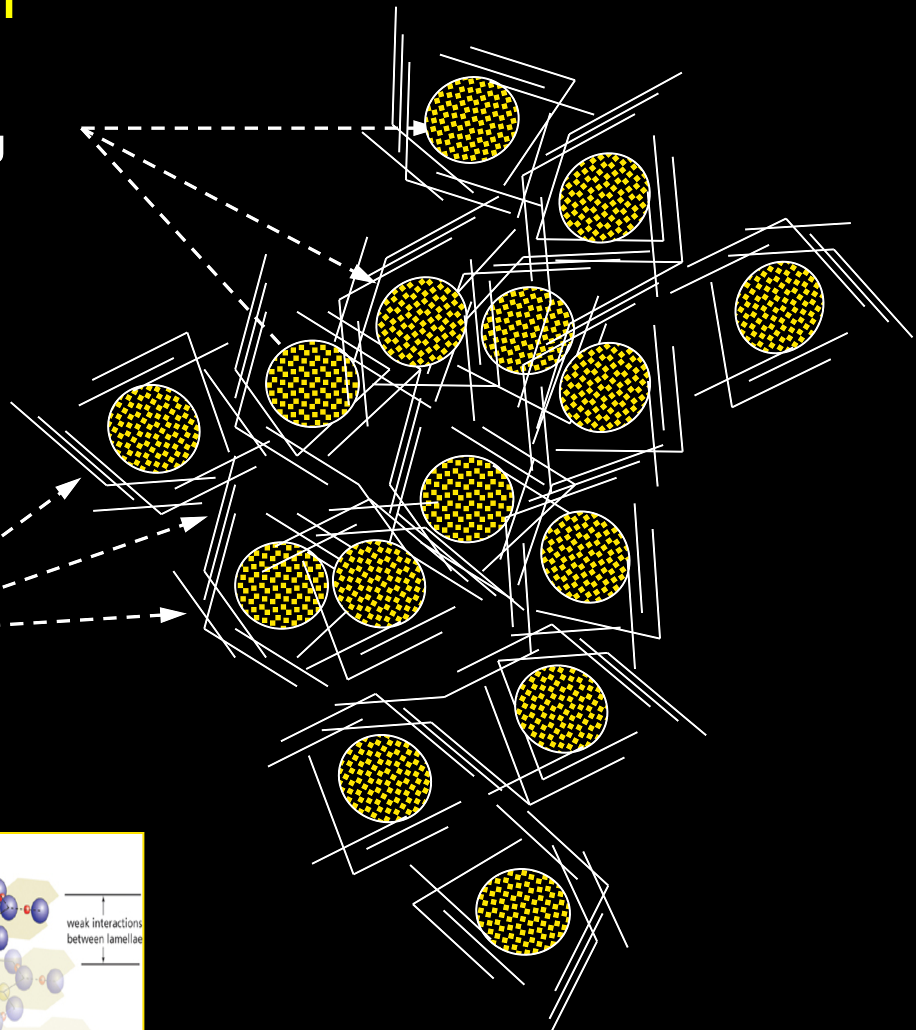
$L \approx 1$cm

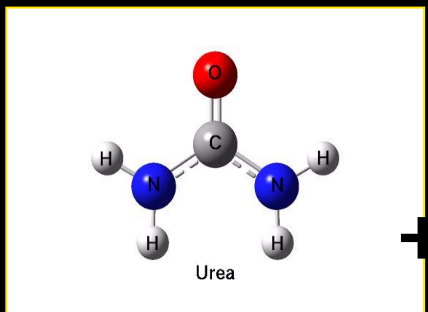
Tubular open tunnels



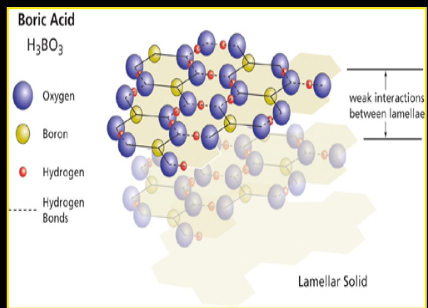
Asbestos host matrix
(Kumzerov & al, 2003)

NANO: LOCALIZATION & CONFINEMENT –Surface Tension





+

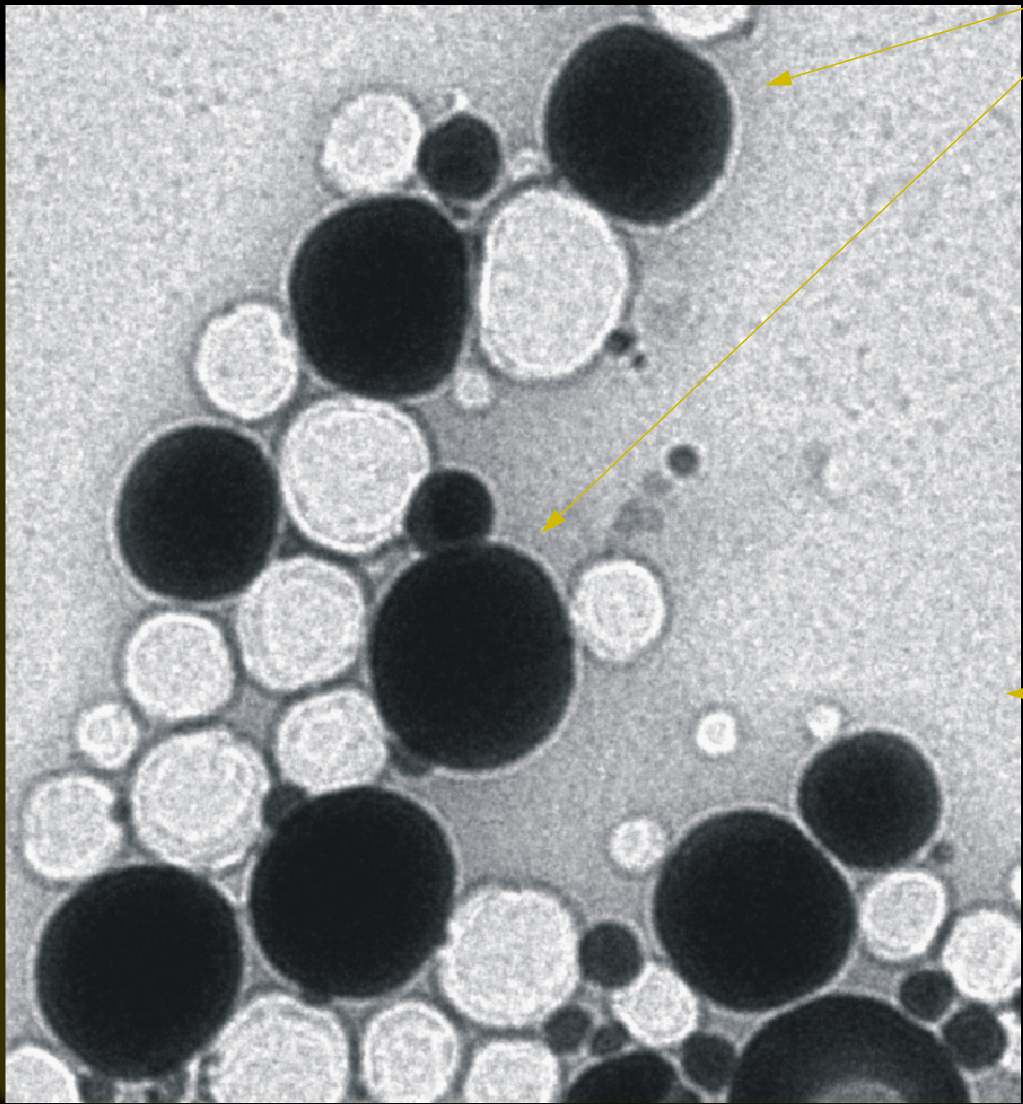


$+_{X}$ $Hg(C_2H_3O_2)$

NANO: LOCALIZATION & CONFINEMENT

–Surface Tension

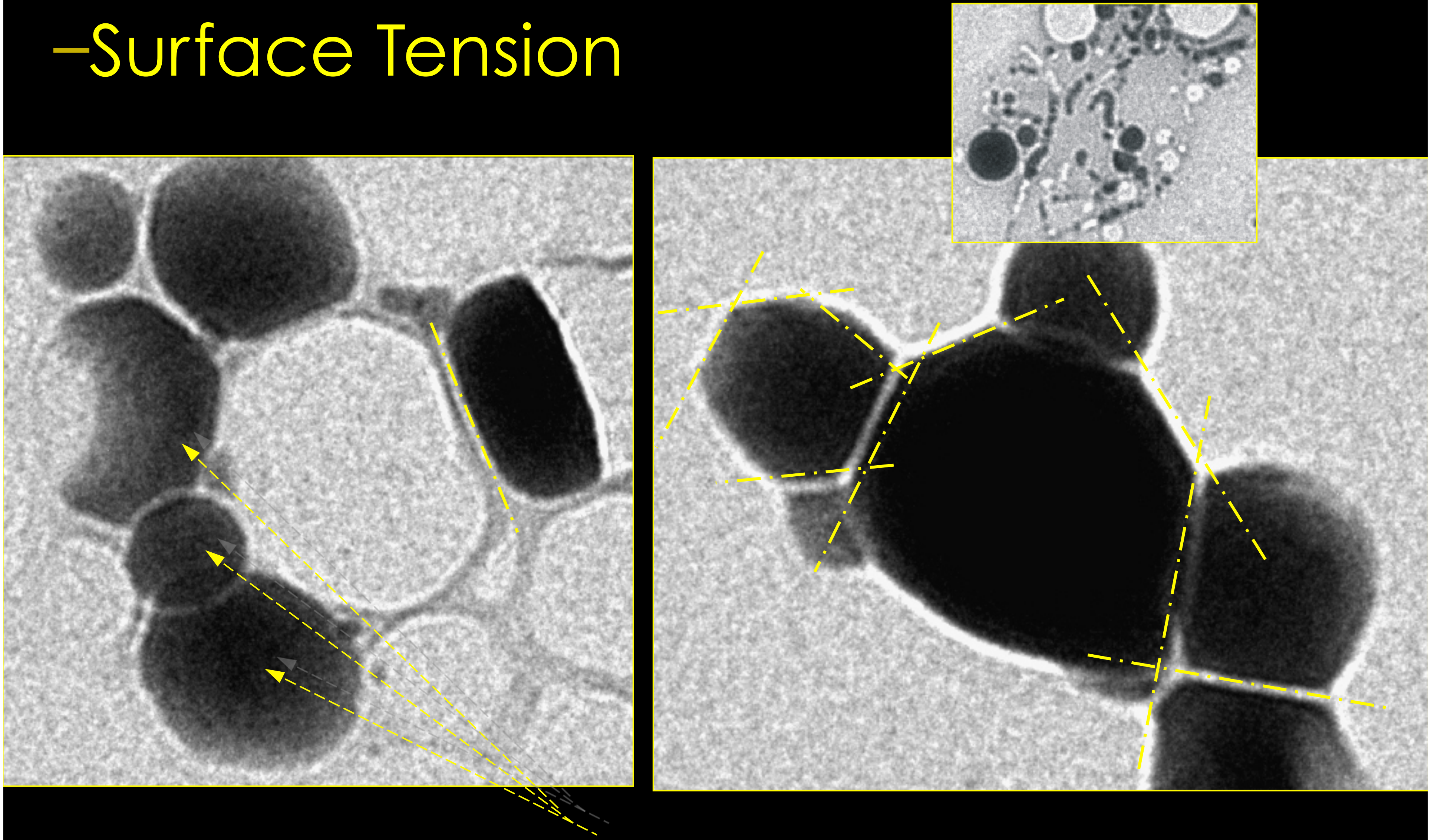
NANO: LOCALIZATION & CONFINEMENT –Surface Tension



$\phi >> 3$ nm

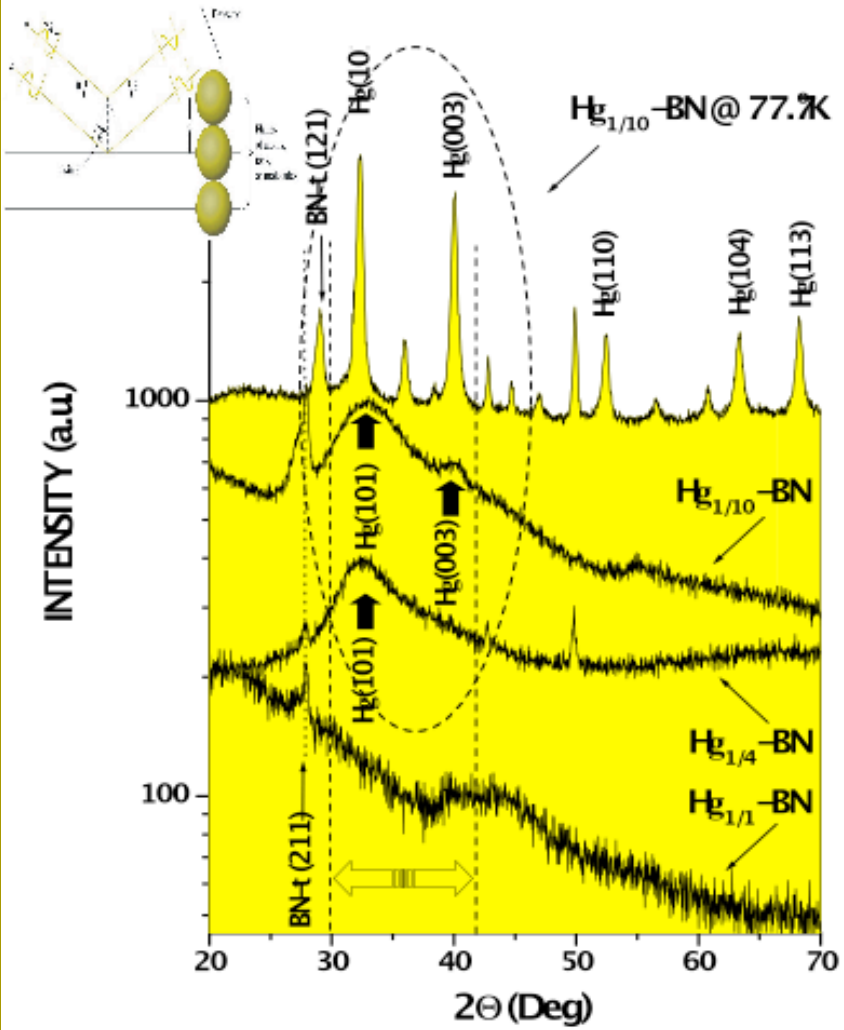
NANO: LOCALIZATION & CONFINEMENT

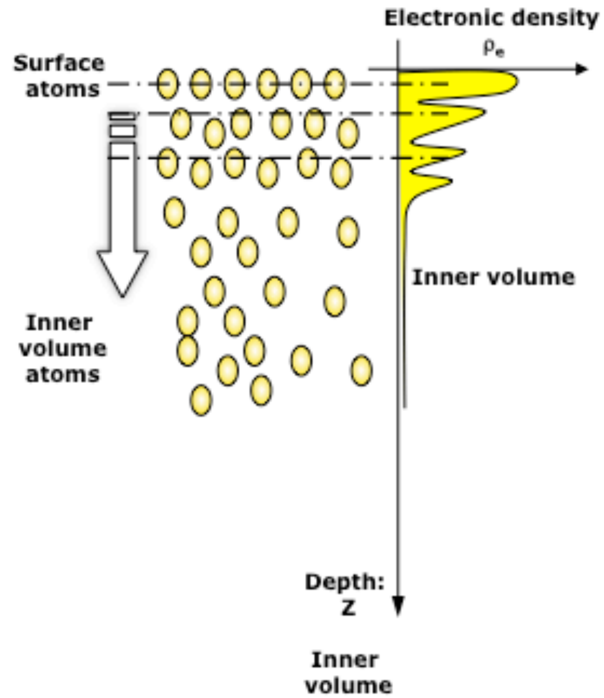
–Surface Tension



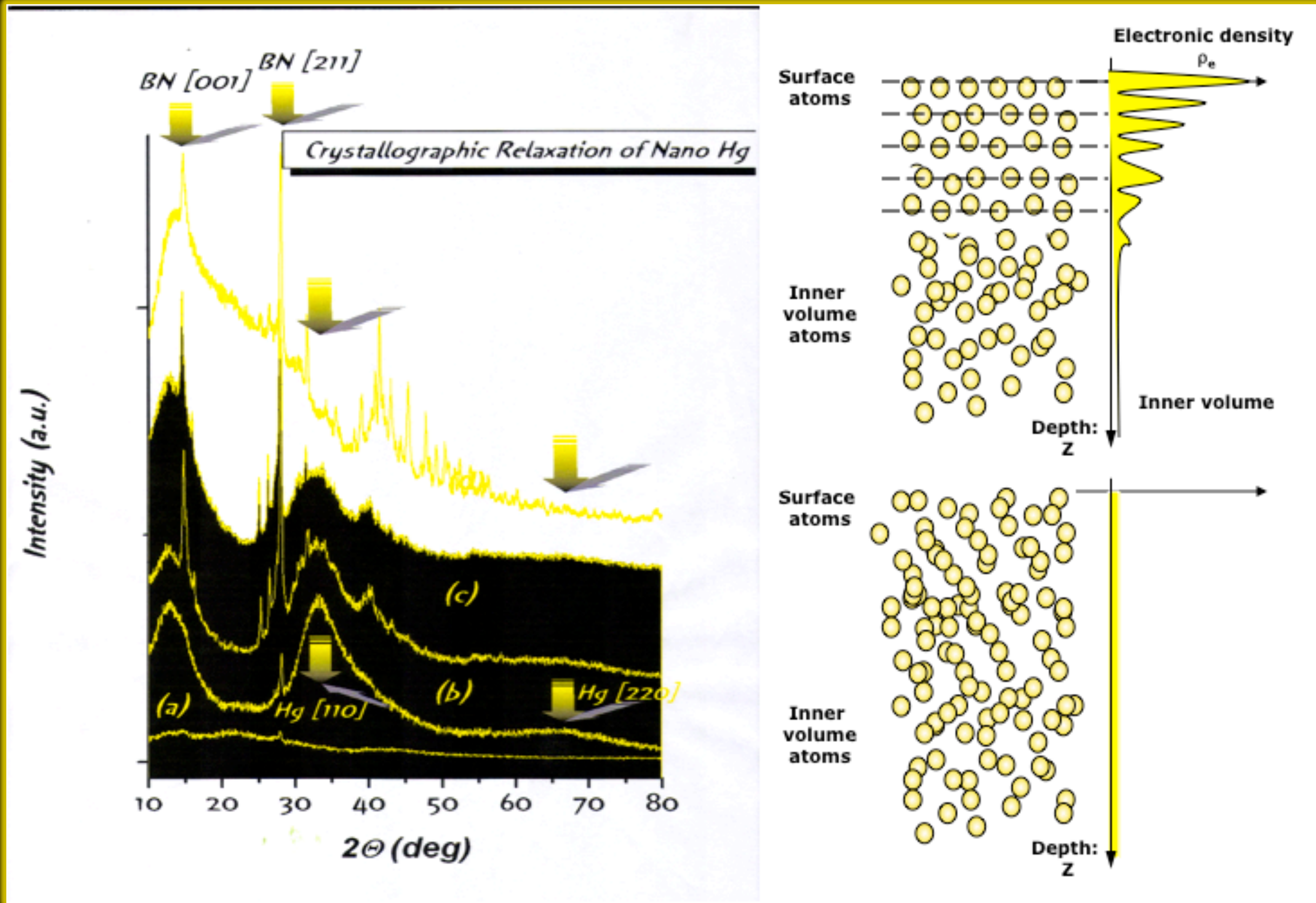
ϕ ≤ 3 nm

NANO: LOCALIZATION & CONFINEMENT –Surface Tension





NANO: LOCALIZATION & CONFINEMENT –Surface Tension



NANO-SCALED SYSTEMS: LOCALIZATION & CONFINEMENT

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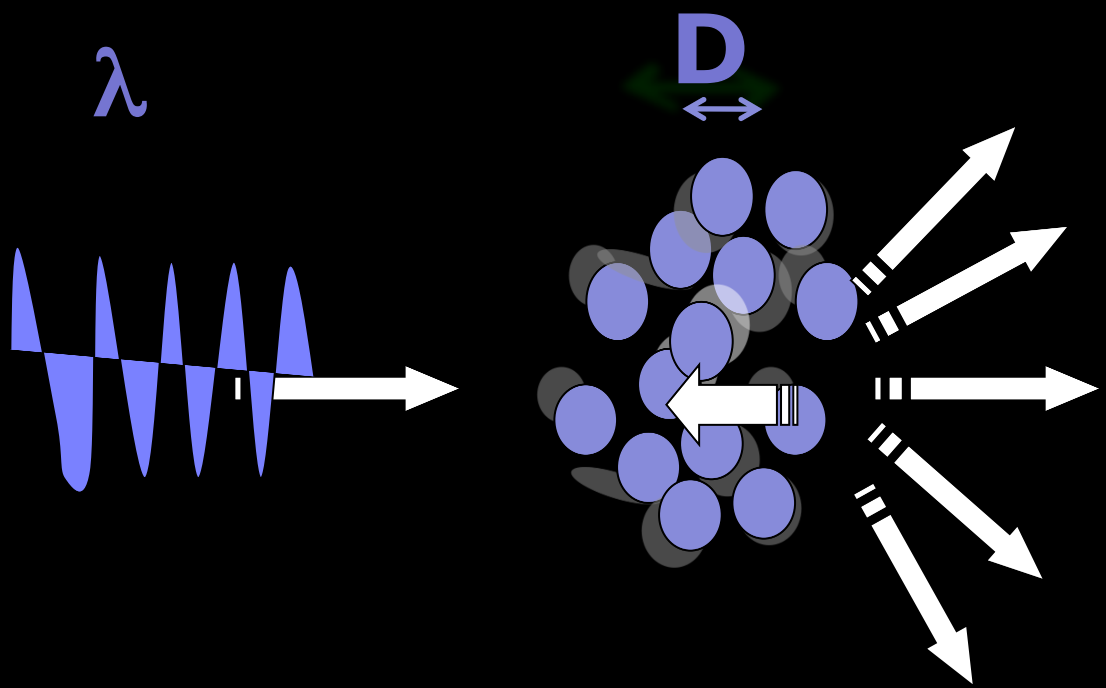
NANO: LOCALIZATION & CONFINEMENT –Anderson Localization



≠ Scattering cases

•Rayleigh type

σ α 1/ λ [4], D< l

•Mie type

D≅ λ , not analytically solvable for arbitrarily shapes

•Anderson loc.:
½ disordered syst.
Random walk type

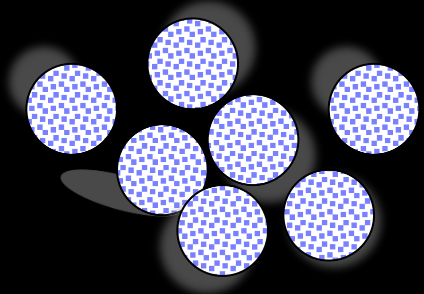
NANO: LOCALIZATION & CONFINEMENT –Anderson Localization

•e wave-packet localization“Anderson, 1958”,
ŸScaling theory of localization “Brahams, 1979”,
ŸMicrowave localiz. by 2-D “Dalichaouch, 1991”,
ŸLight localiz. in disordered Sys “Wiersma, 1997”,
ŸLight localiz. By cold atoms “Labeyrie, 1999”,
ŸMultiple light scattering by atoms “Kaiser, 2000”,
ŸLasing in disordered media“Cao, 2000”,
ŸNanowire lasers“Maslov, 2003”,
ŸOptical necklace states 1-D “Bertolotti,2005”,
ŸLasing in single nanowire “Agarwal, 2005”,
ŸAnderson loc. In CNTs“Maaza & al, 2007”.

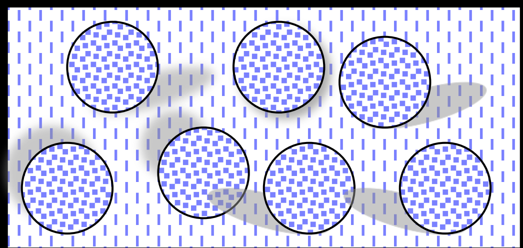
NANO: LOCALIZATION & CONFINEMENT

–Anderson Localization

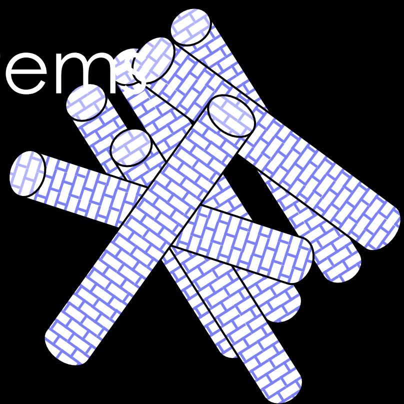
1-Free naoparticles



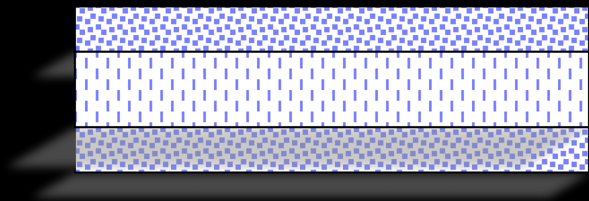
2-Nano-composites



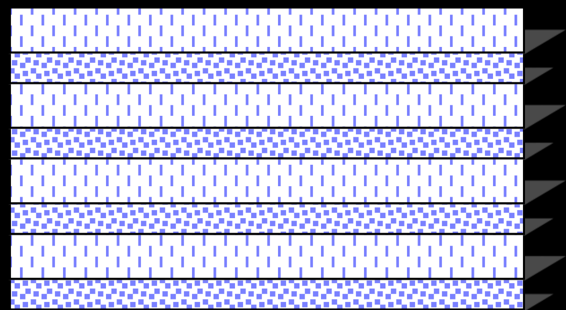
3-nano-Tubular systems



4-Nano-sandwich systems



5-Nano-Multilayered systs.



NANO: LOCALIZATION & CONFINEMENT –Anderson Localization

•CNTs SHAPE ANISOTROPY : Exploration as

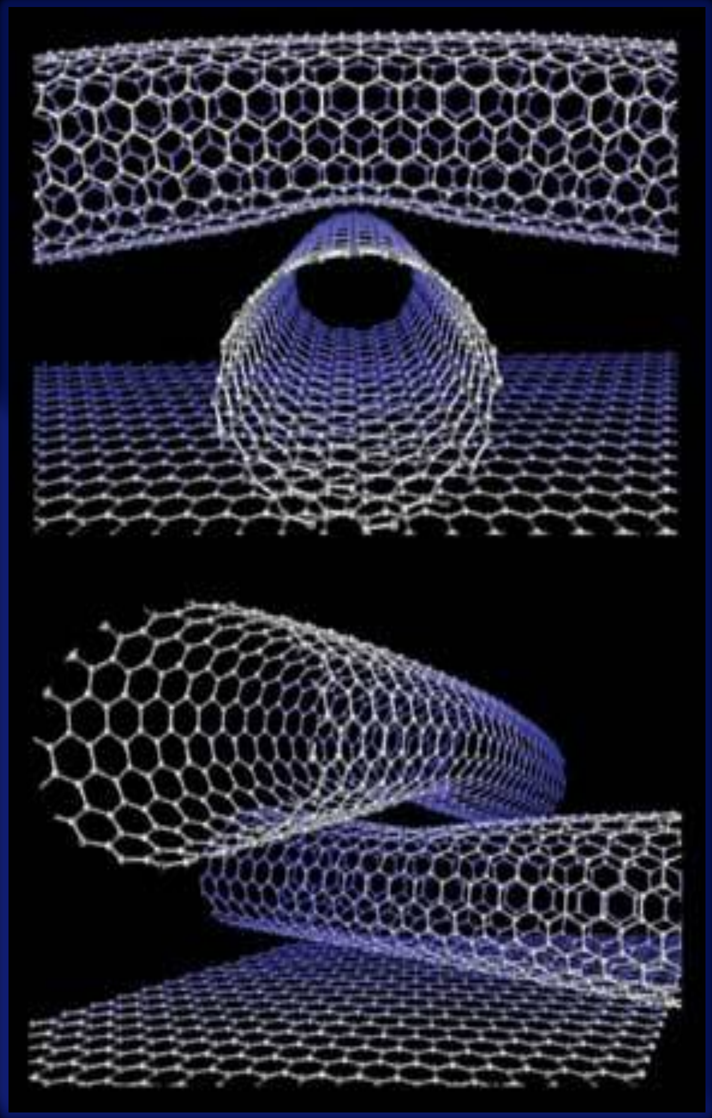
•Alternative to crystal lattice for particles channeling guiding/ 0.34 nm free space between graphitic sheets/ still ≈2 standard crystal lattice

•Possible new source for Hard X-rays

"Letokhov, PLA 2002"

•Highly directional γ-rays source for selective photo-nuclear reactions

"Letokhov, PLA.2003-Artru, PRL.2004"



NANO: LOCALIZATION & CONFINEMENT –Anderson Localization

•Semi-Disordered media, the transport of light with wavelength "l" depends strongly on the length scales of the system. Relevant scales are the transport mean free path "ξ" the distance after which the propagation direction of light is randomized & sample thickness "D".

•3 main scattering processes can take place in such Semi-Disordered media with total transmission "T": .

(i) Diffusive scattering in non –absorbing medium: $\lambda<\xi<<D$, $T\cong \xi/D$

(ii) Weak Anderson Loc.: $2\pi\xi/\lambda \rightarrow 1$, $T\cong 1/D^2$

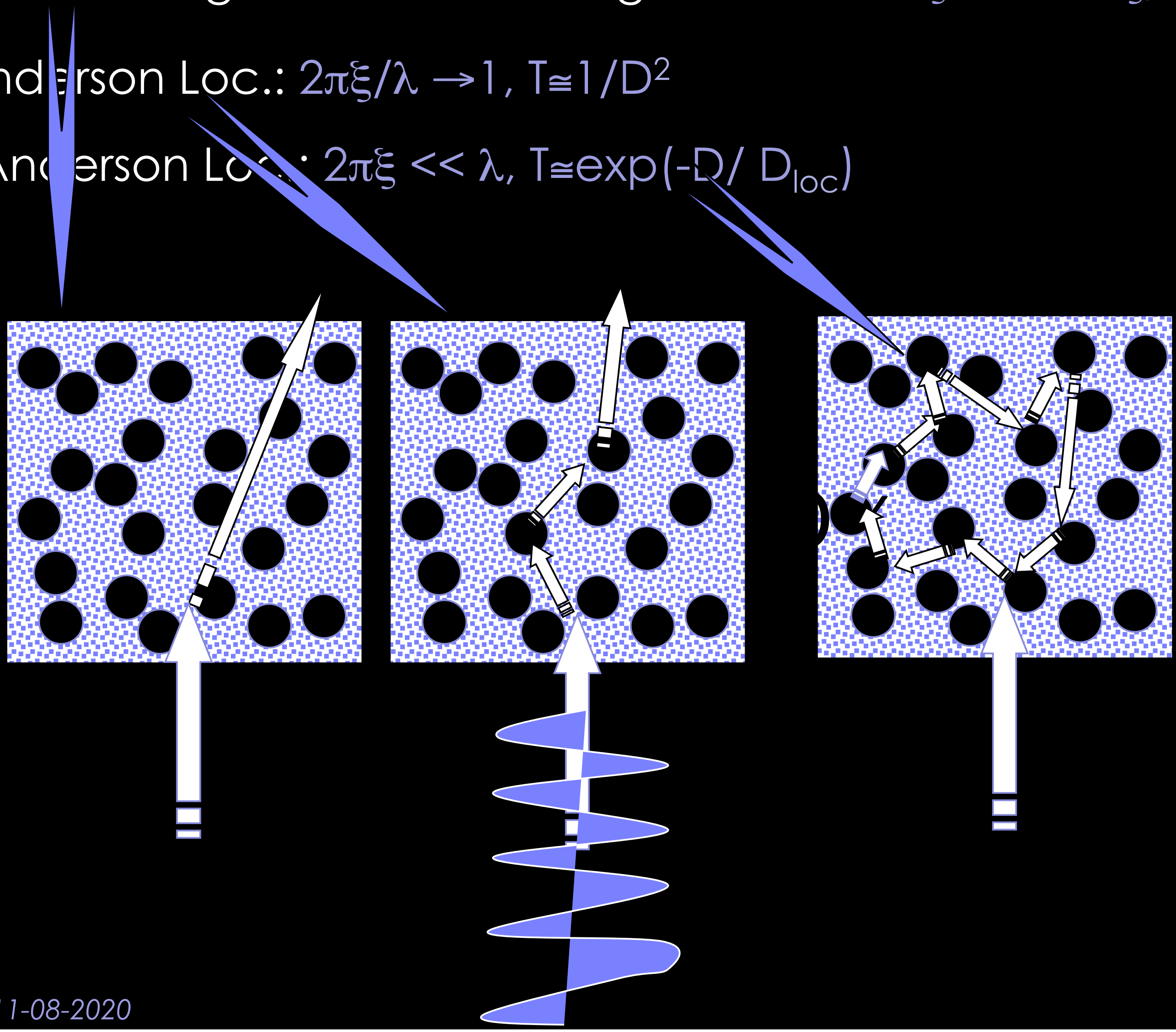
(iii) Strong Anderson Loc.: $2\pi\xi << \lambda$, $T\cong \exp(-D/ D_{loc})$

NANO: LOCALIZATION & CONFINEMENT

(i) Diffusive scattering in non –absorbing medium: $\lambda<\xi<<D$, $T\cong \xi/D$

(ii) Weak Anderson Loc.: $2\pi\xi/\lambda \rightarrow 1$, $T\cong 1/D^2$

(iii) Strong Anderson Loc.: $2\pi\xi << \lambda$, $T\cong \exp(-D/ D_{loc})$



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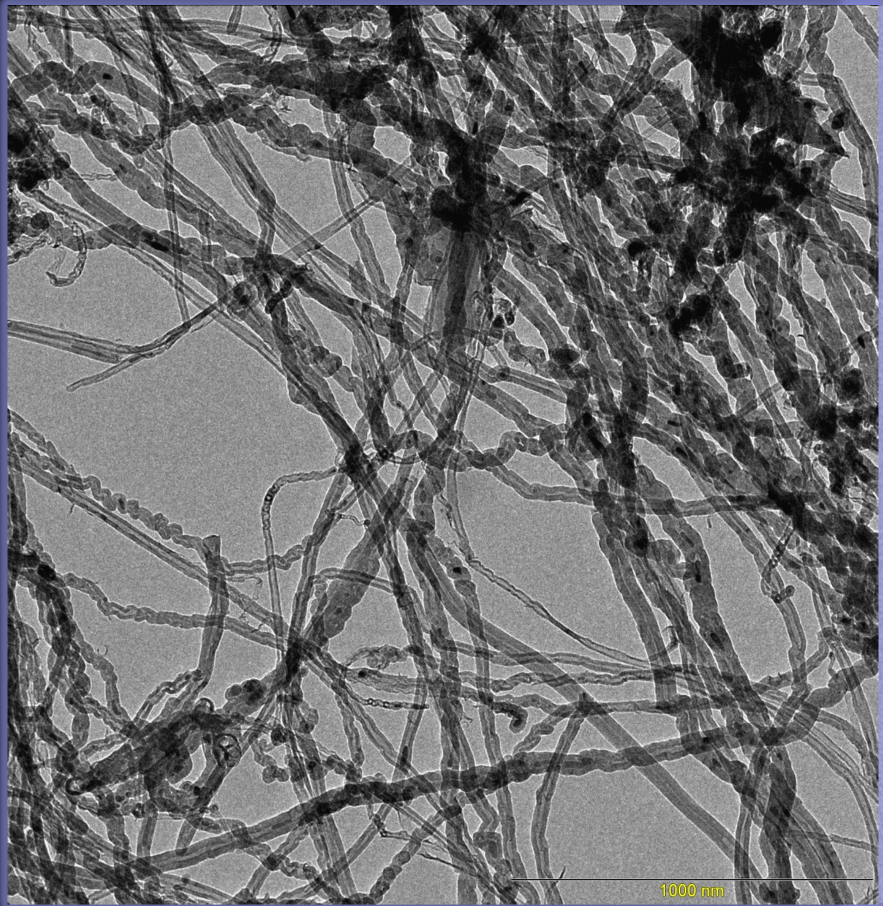
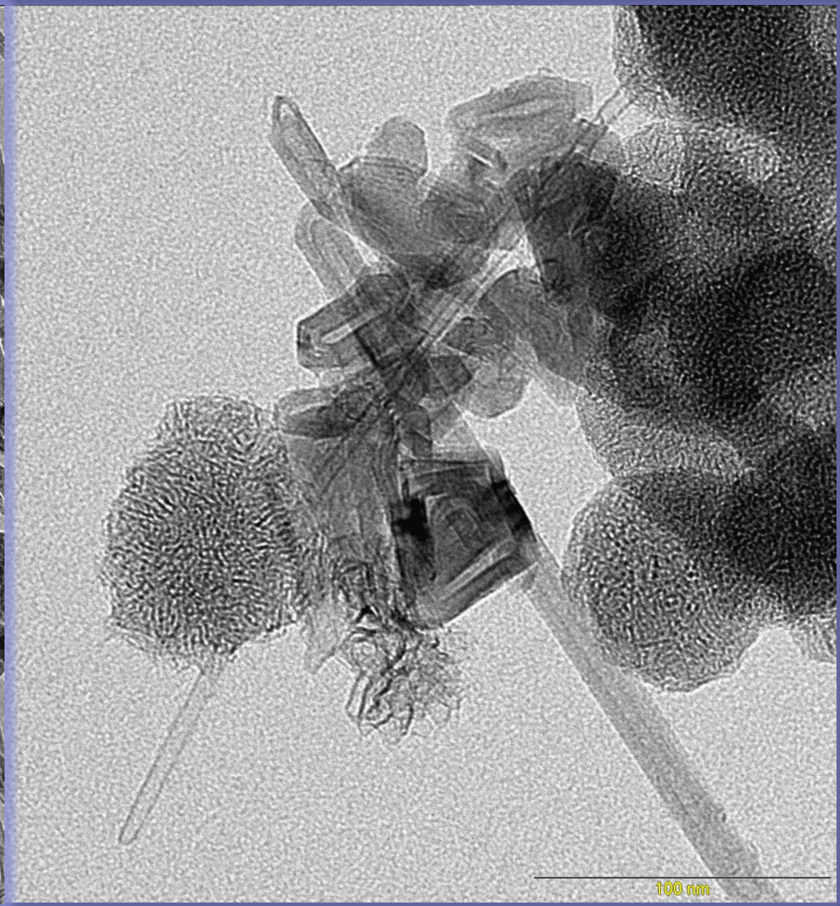
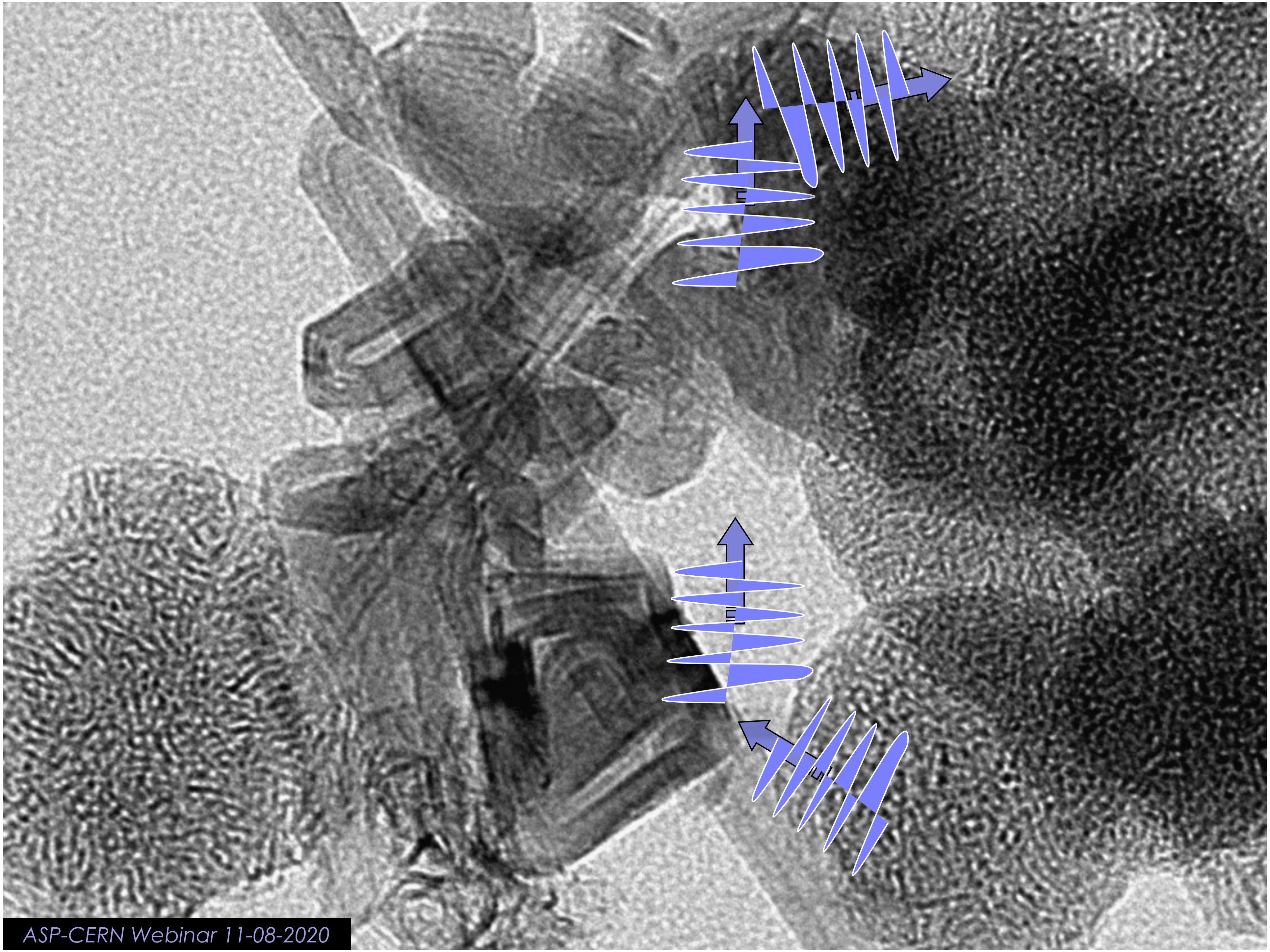




Spaghetti-type

Ship-shaped type



NANO: LOCALIZATION & CONFINEMENT –Anderson Localization

- $E_z = E_0 \exp(-z/\xi_{Depth})$
- $\xi_{Depth} = (\lambda/2\pi n_{Crys})(\sin^2\theta - (n_{CNTs}/n_{Cryst})^2)^{1/2}$

•Germanium crystal:

-$n_{Ge} \approx 4.0$ in IR-FIR

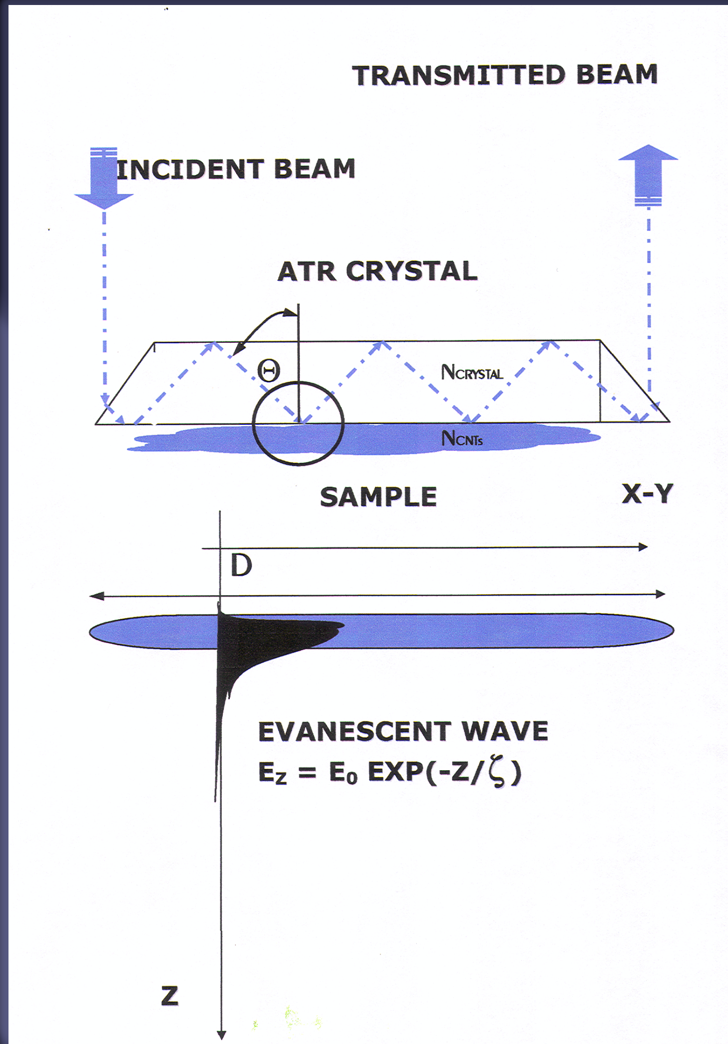
- ξ_{Depth} (σ= 1000cm^{-1})=

-ZnSe: 1.66 μm

-AMTIR: 1.46μm

-Ge: 0.65μm

•High rupture modulus: 7 10^3Psi



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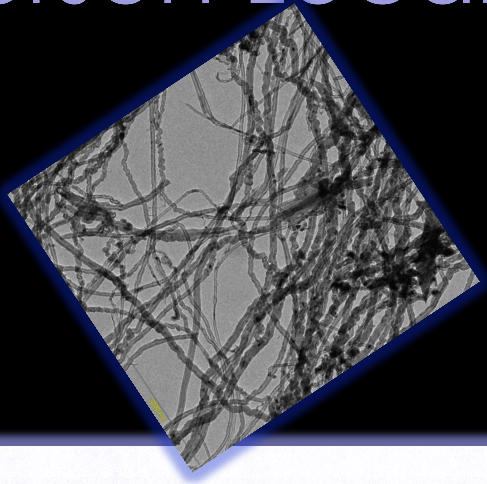
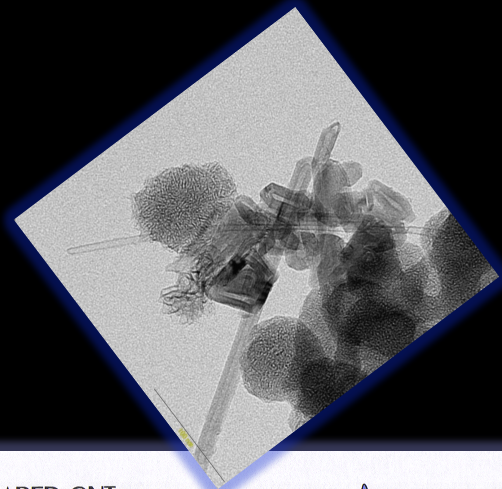
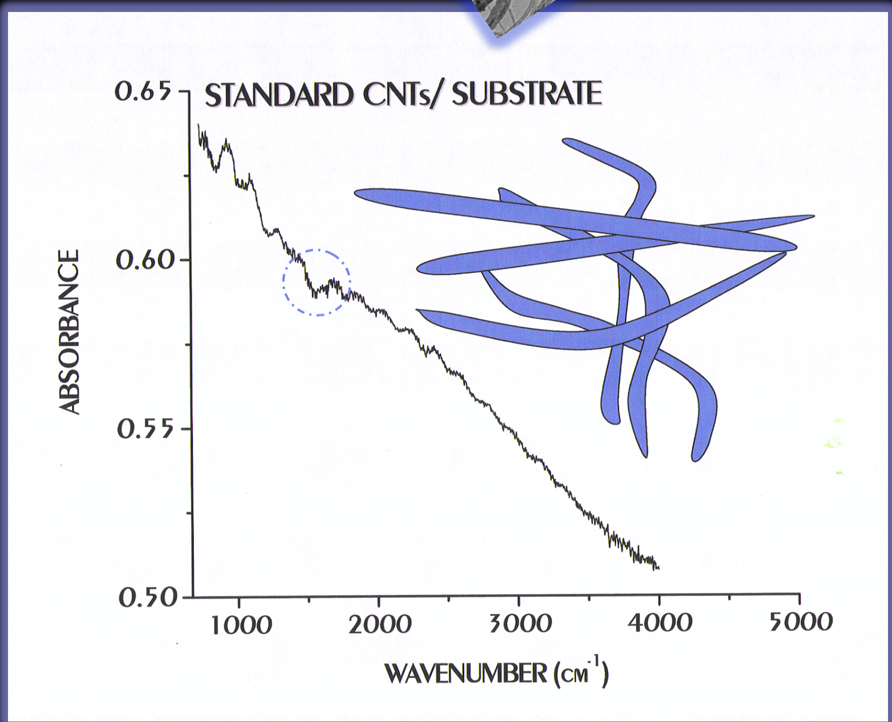
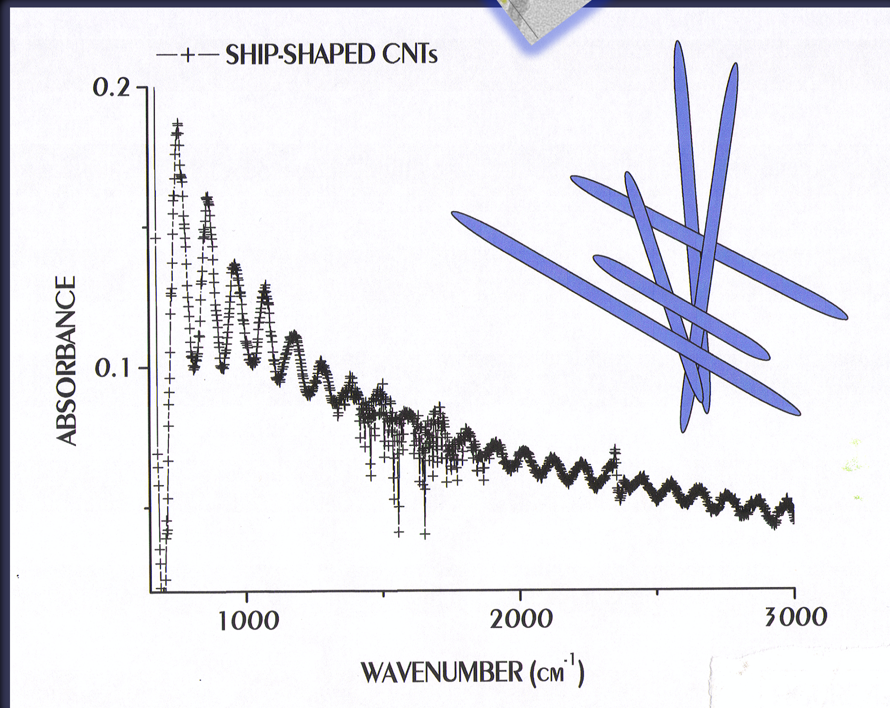
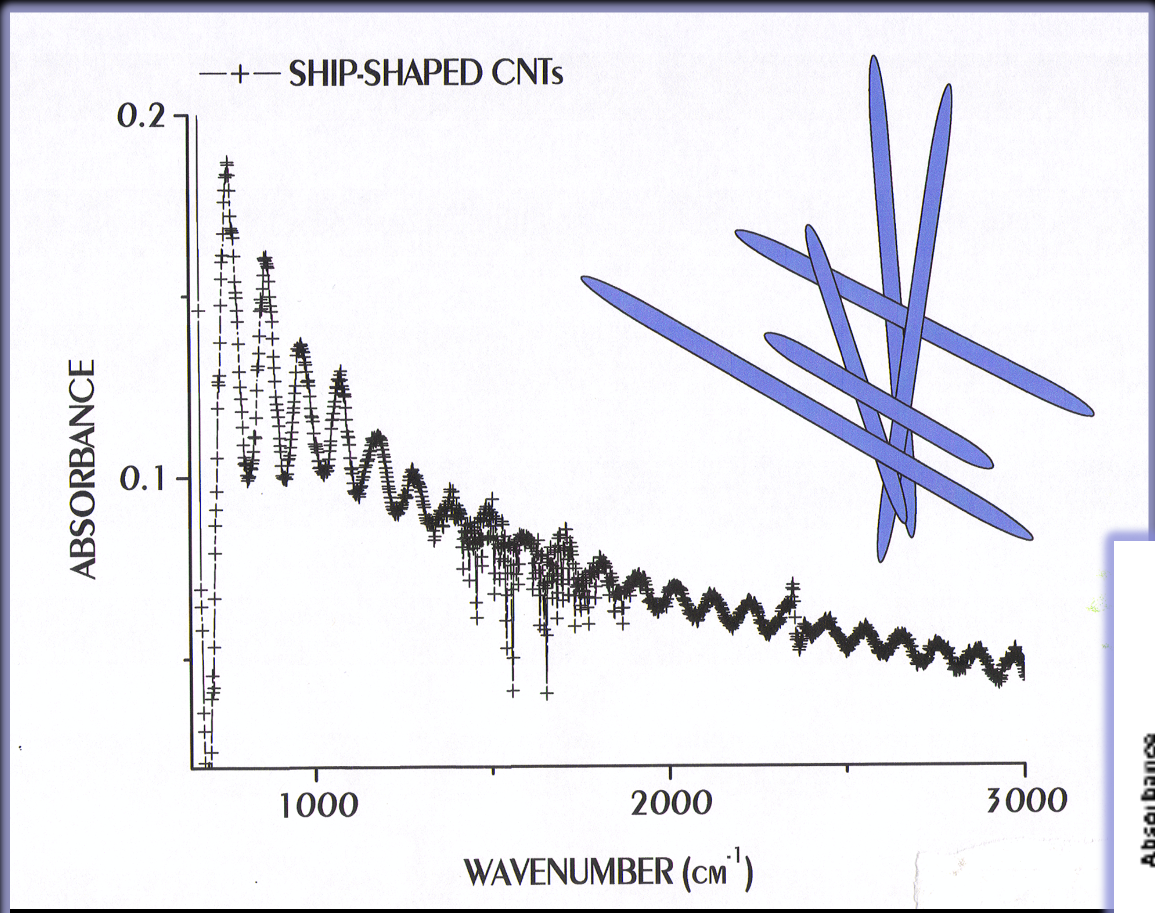


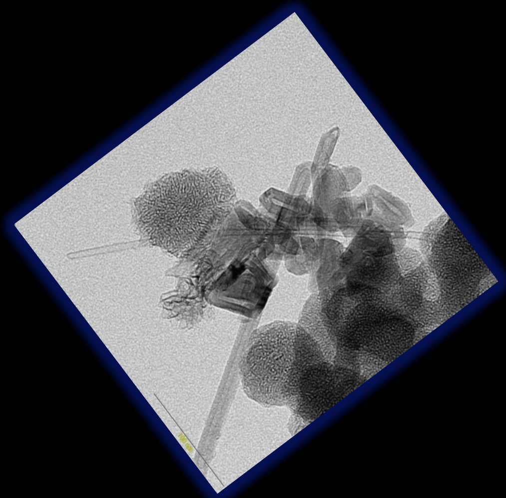


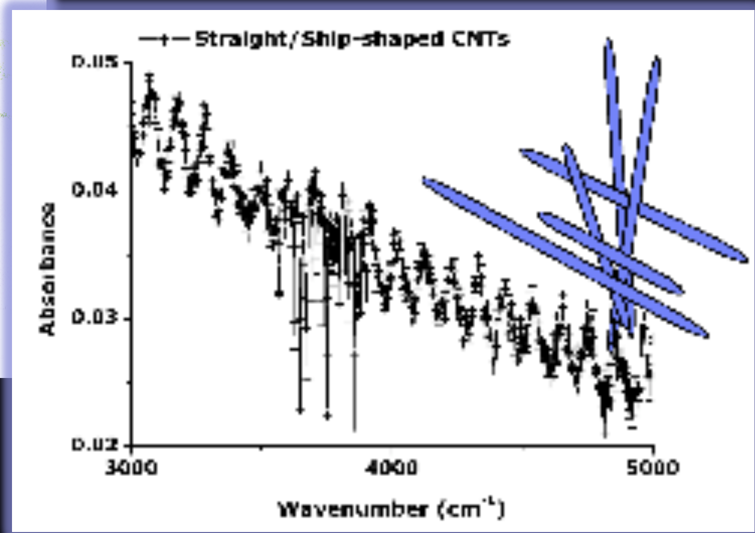




NANO: LOCALIZATION & CONFINEMENT –Anderson Localization



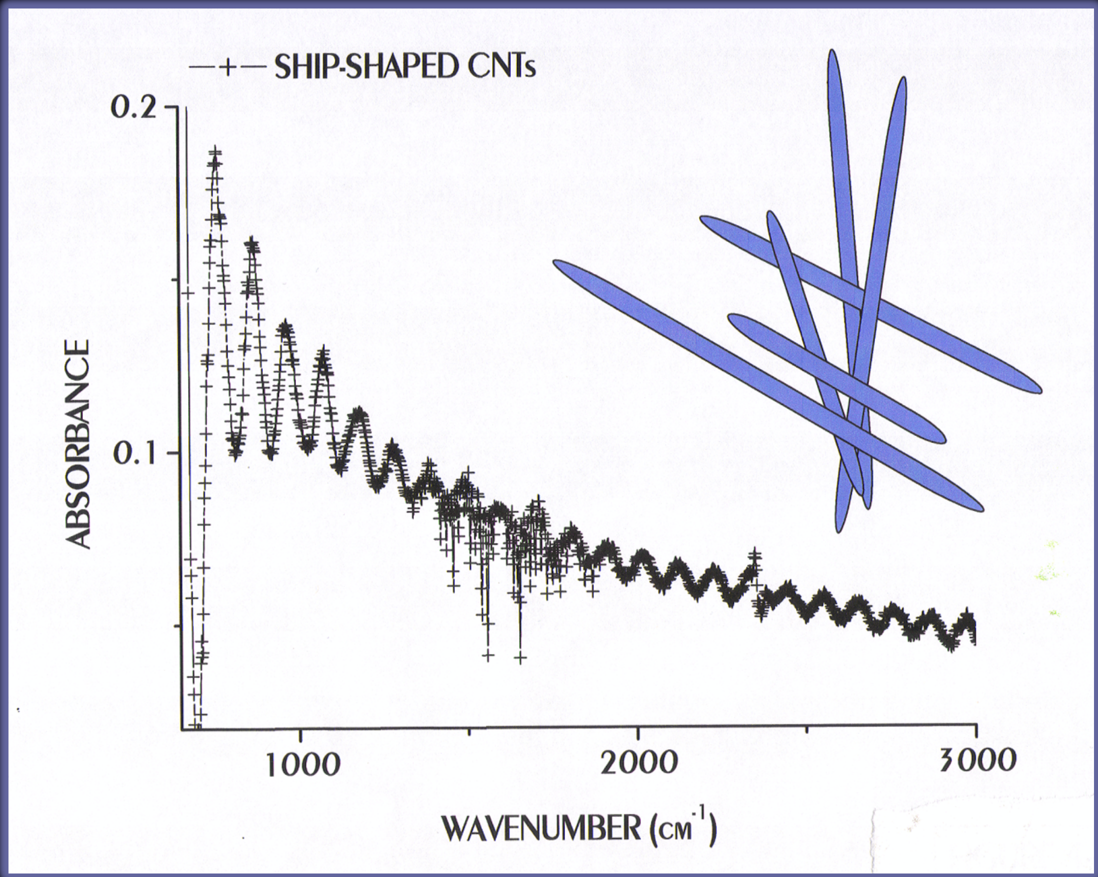


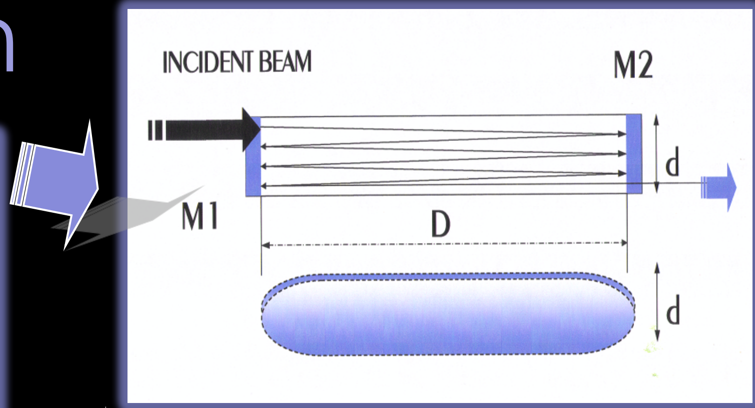


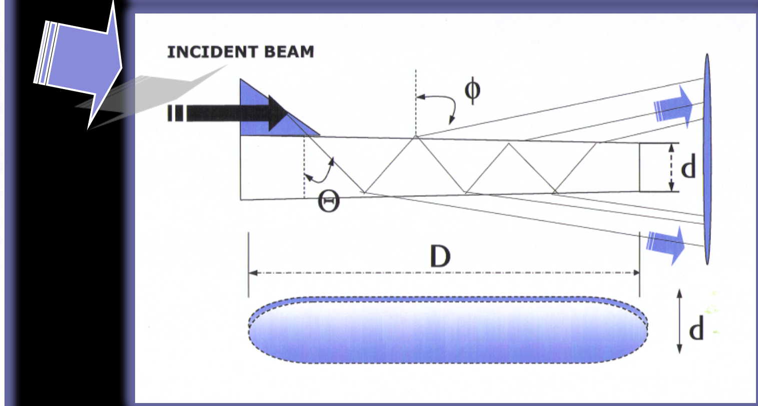
- Interference: ≅ 40 maxima, $\Delta\sigma$ ≅ 105 cm^{-1}
- Envelope: Exponential decay

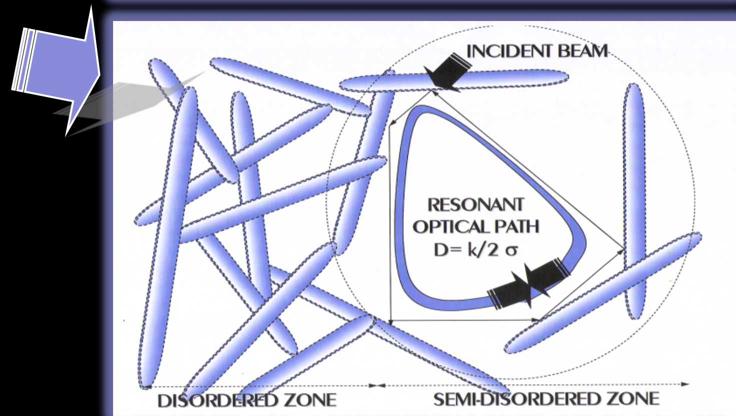
NANO: LOCALIZATION & CONFINEMENT

–Anderson Localization

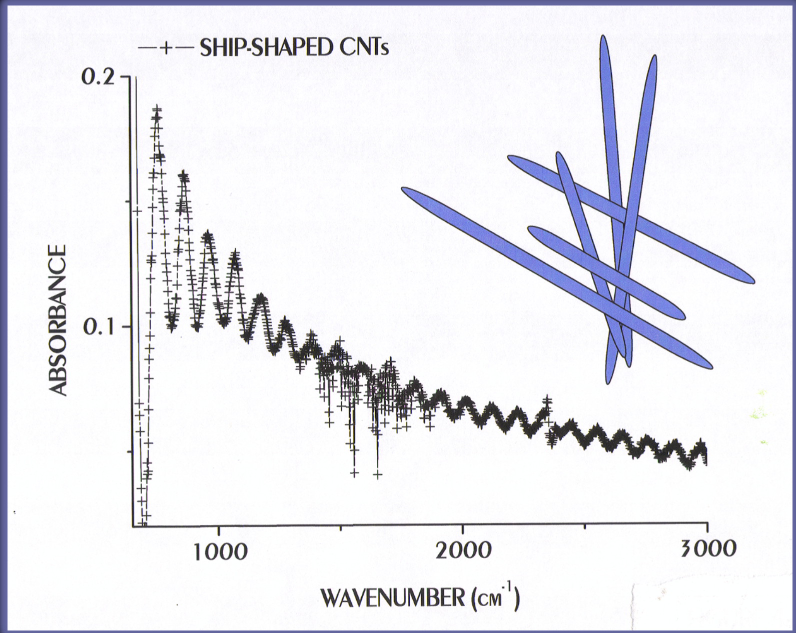


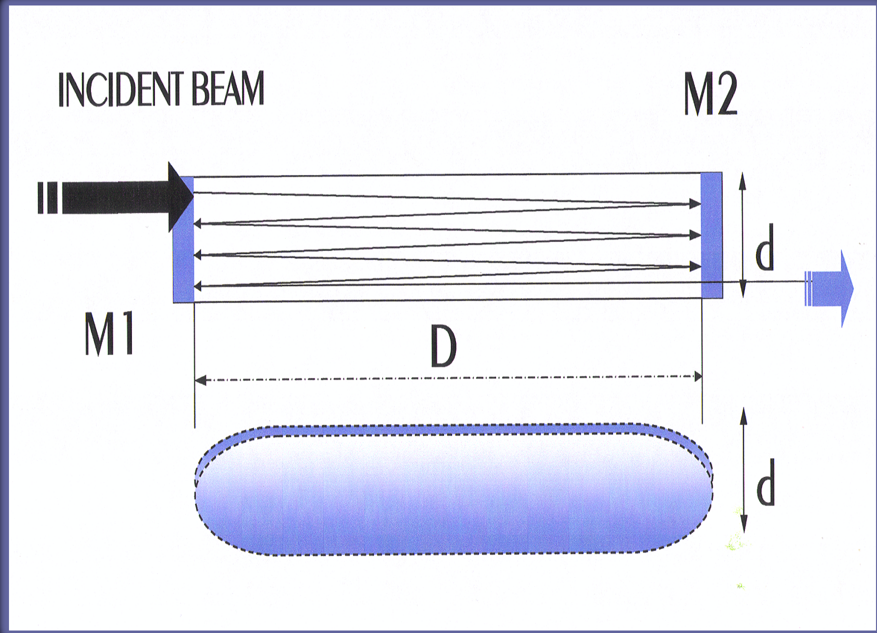






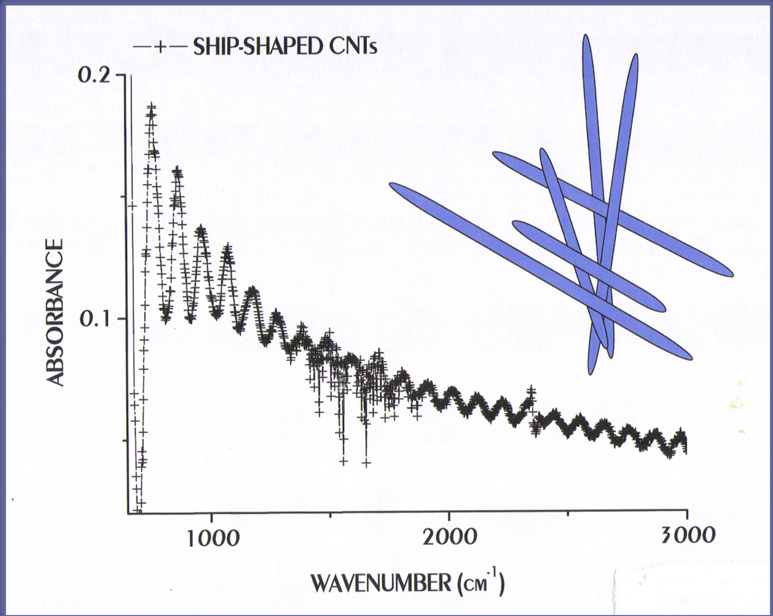
NANO: LOCALIZATION & CONFINEMENT –Anderson Localization

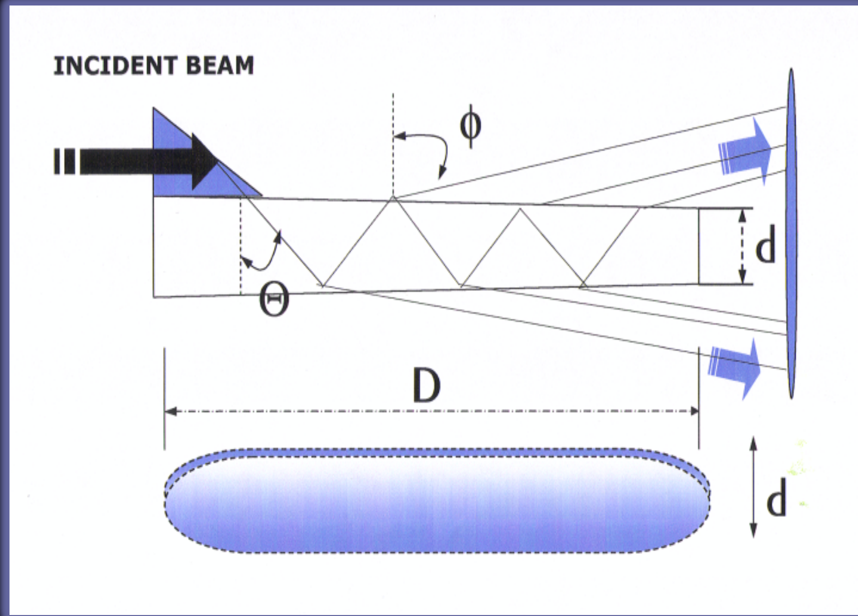




- $\sigma_k = \frac{1}{2}\ k\ n_{Cav}\ D_{Cav}$
- $\Delta\sigma = \frac{1}{2}\ n_{Cav}\ D_{Cav} \cong 105\ cm^{-1}$: $D_{Cav} \approx 47\mu m$/ $<L_{CNTs}>0.6\text{-}3.7\ \mu m$
- $R = (\Delta\sigma_{HWHM} 2\pi\ n_{Cav} D_{cav}) + \sqrt{((\Delta\sigma_{max} 2\pi\ n_{Cav} D_{cav})^2 + 4))}/2 \approx 66.4\%$!!

NANO: LOCALIZATION & CONFINEMENT –Anderson Localization



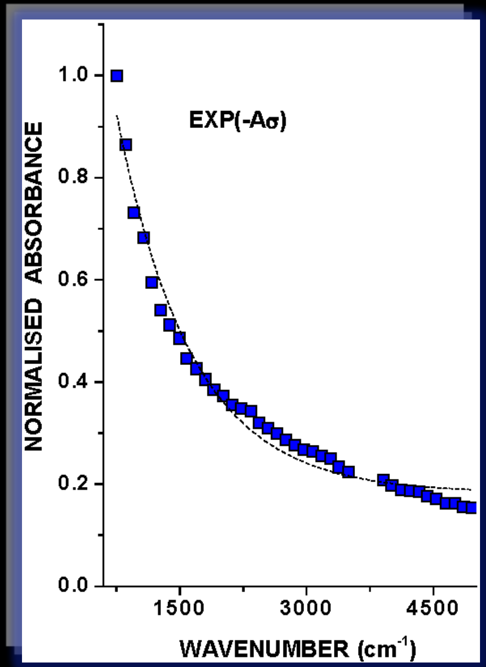


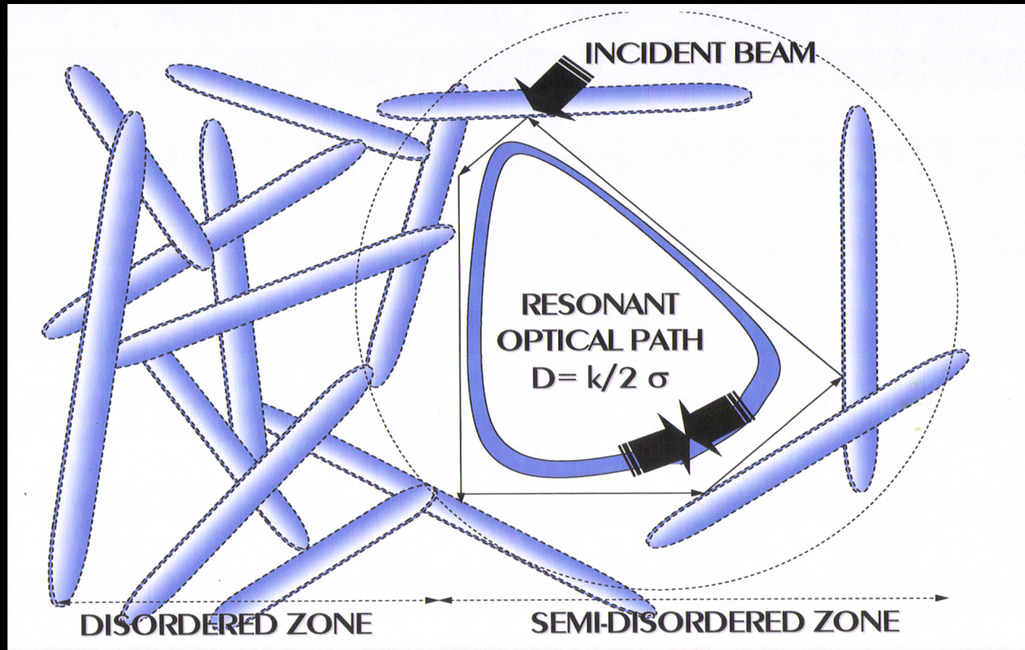
- $\sigma_k = ½ \; k\,(n^2_{Cav} - \sin^2\phi)$
- TEM: $\langle L_{CNTs} \rangle$0.6-3.7 μm, Transversal≈ 1-15 graphitic layers

$\Delta\sigma \approx$ 7-52 10^7 cm^{-1} !!!!

$\Delta\sigma_{Exp} \approx$ 150-185 cm^{-1}

NANO: LOCALIZATION & CONFINEMENT –Anderson Localization





→ As the absorption maxima with an exponential decaying envelope, occurs at equal $\Delta\sigma$, it might be generated by a resonating cavity of an optical length n_{CAV} D_{CAV} ; $D_{CAV} \approx 46.7$ μm due to the ship-shaped CNTs (0.06- 3.7 μm long): signature of a strong Anderson localization.

NANO: LOCALIZATION & CONFINEMENT –Anderson Localization

638 *Int. J. Nanotechnol., Vol. 4, No. 6, 2007*

On the possible optical resonance in carbon nanotubes based cavities

Localization of light in a disordered medium

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Journal of Statistical Physics, Vol. 76, pp. 985-1003, 1994

Localization of Electromagnetic and Acoustic Waves in Random Media. Lattice Models

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NANO: LOCALIZATION & CONFINEMENT –Anderson Localization

On the possible optical resonance in carbon nanotubes based cavities

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On the possible optical resonance in carbon nanotu

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Abstract: An enhanced interference phenomenon in
wavenumber profiles of ship-shaped carbon nanotube
observed by attenuated total reflection at room tem
temperature interference phenomenon was considered a
from an optical resonance effect and that single carb
act as individual Fabry-Perot or Lummer-Gehrcke re
demonstrated that this interference phenomenon cou
type localisation phenomenon due to resonant modes i
ship-shaped carbon nanotubes nanopowder which cou
resonant cavity.

Keywords: carbon nanotubes; attenuated total reflectio
cavity; infrared spectroscopy; multiple scattering and ran
localisation phenomenon.

Reference to this paper should be made as follows: Maa
Ndwandwe, M.O., Cingo, N., Beye, A.C., Govindaraj,
(2007) 'On the possible optical resonance in carbon nano
Int. J. Nanotechnol., Vol. 4, No. 6, pp.638–650.

Biographical notes: Dr. M. Maaza holds a MSc and PhD
and Photonics at the Nanoscale from Paris VI Universi
include investigation of surface-interface phenomena, low dimensional systems

3 Govindaraj, A. and Rao, C.N.R. (2002) 'Organometallic route to carbon nanotubes', *Pure Appl. Chem.*, Vol. 74, No. 9, p.1571.

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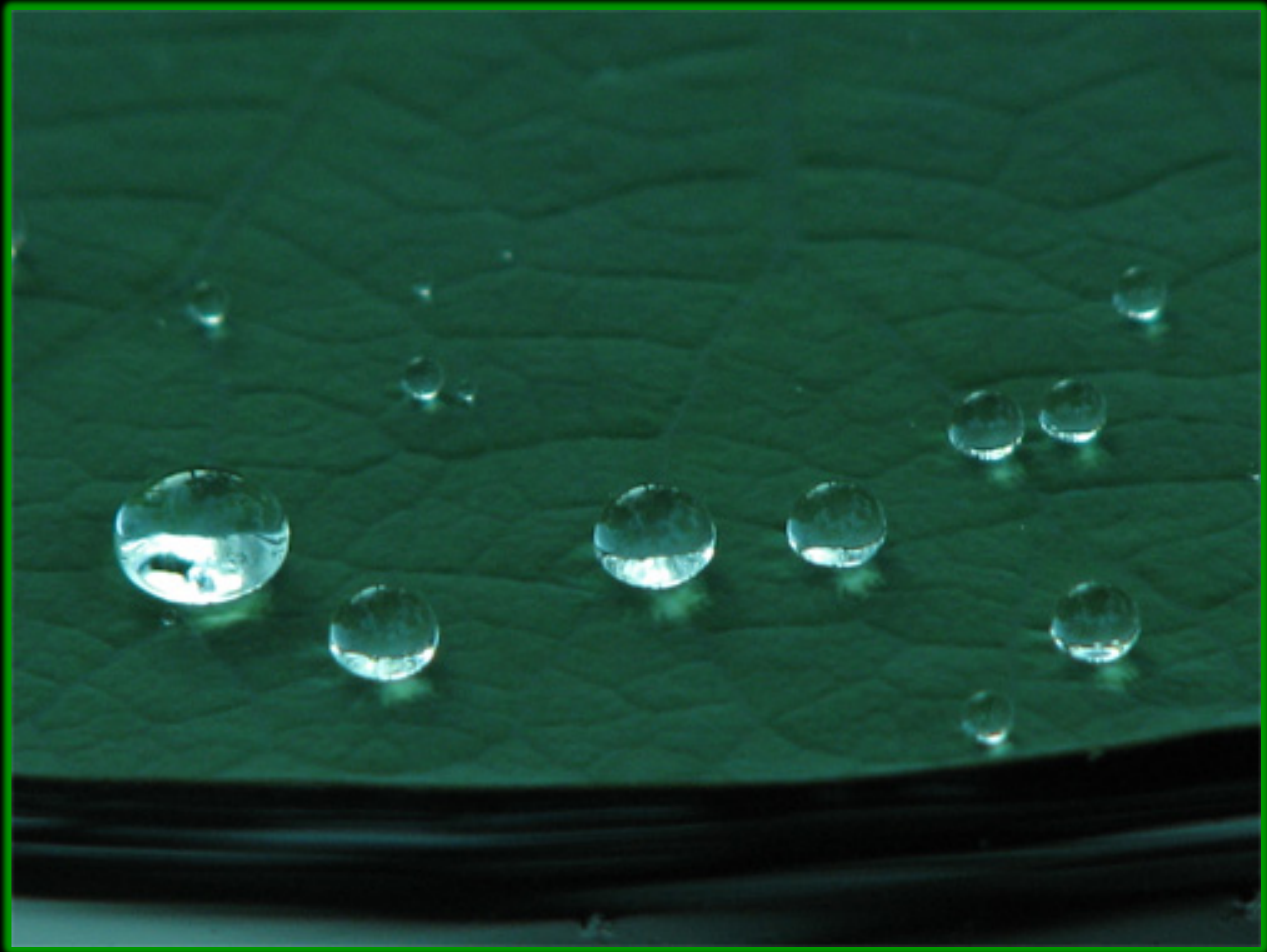
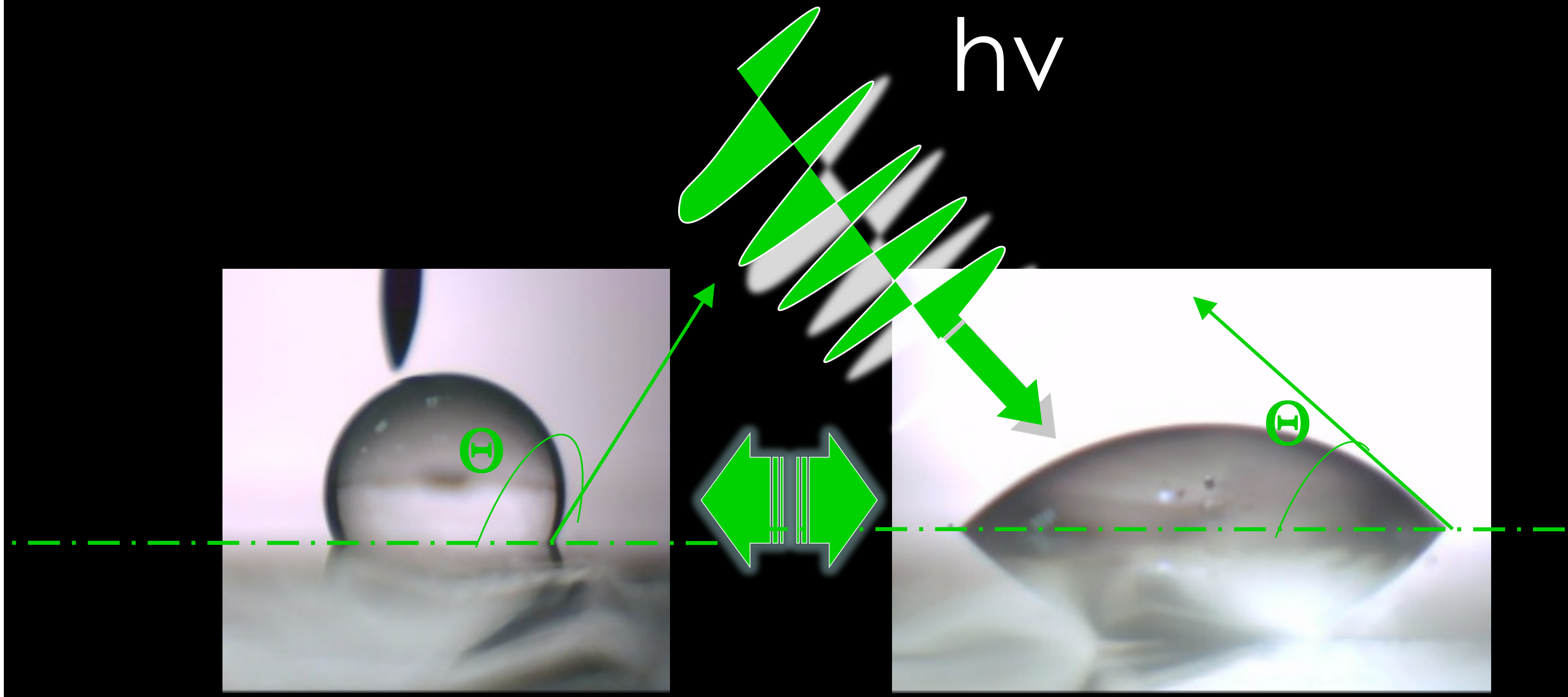
NANO-3:
TUNABLE SURFACE TENSION

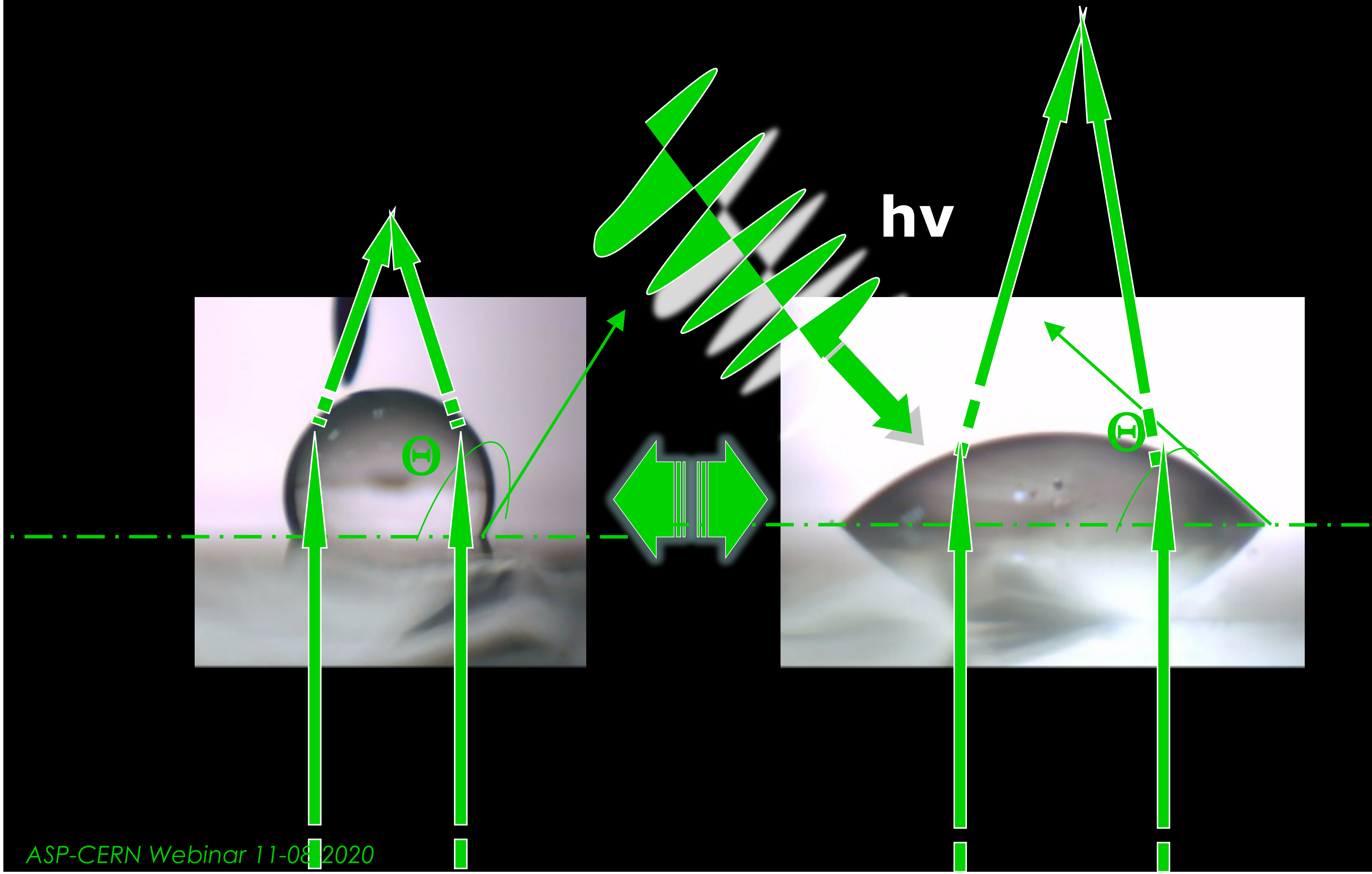


NANO: LOCALIZATION & CONFINEMENT –Surface Tension Tunability



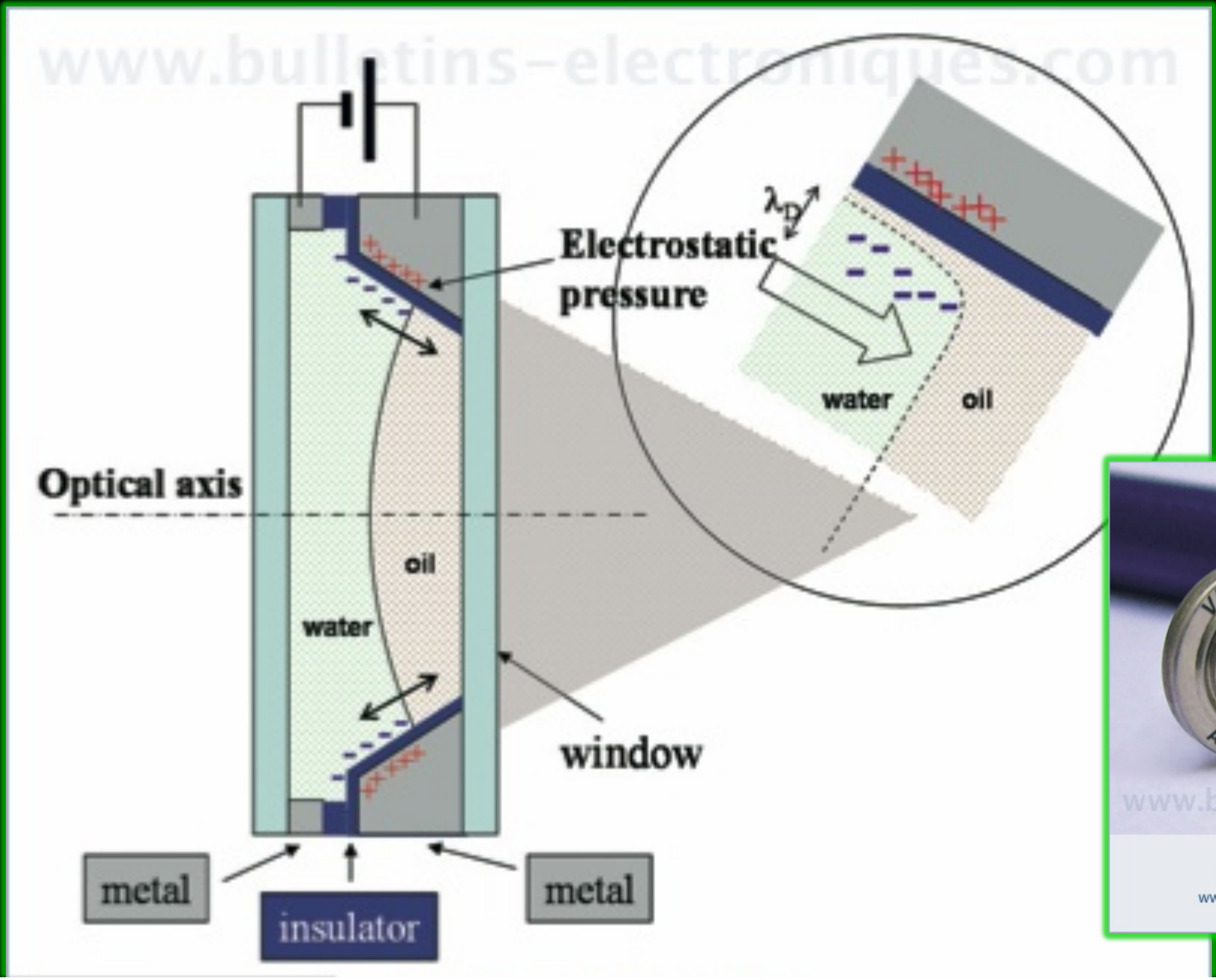
NANO: LOCALIZATION & CONFINEMENT

- Liquid lens with tunable focus "f"



NANO: LOCALIZATION & CONFINEMENT

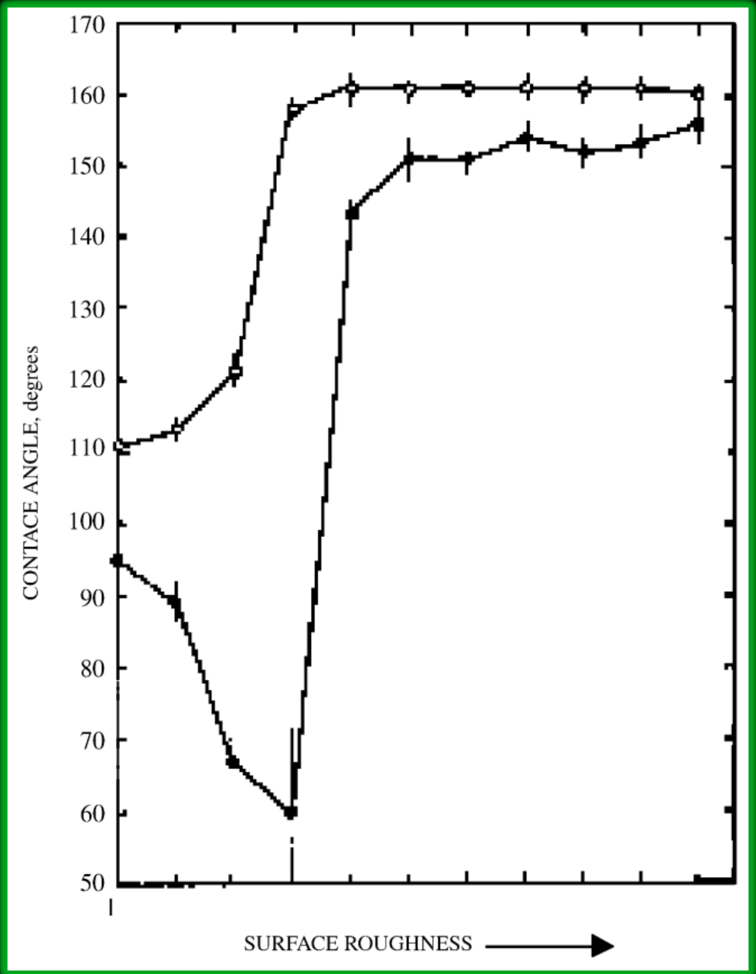
- Liquid lens with tunable focus "f"
- "Varioptic/ Singapore" liquid lens

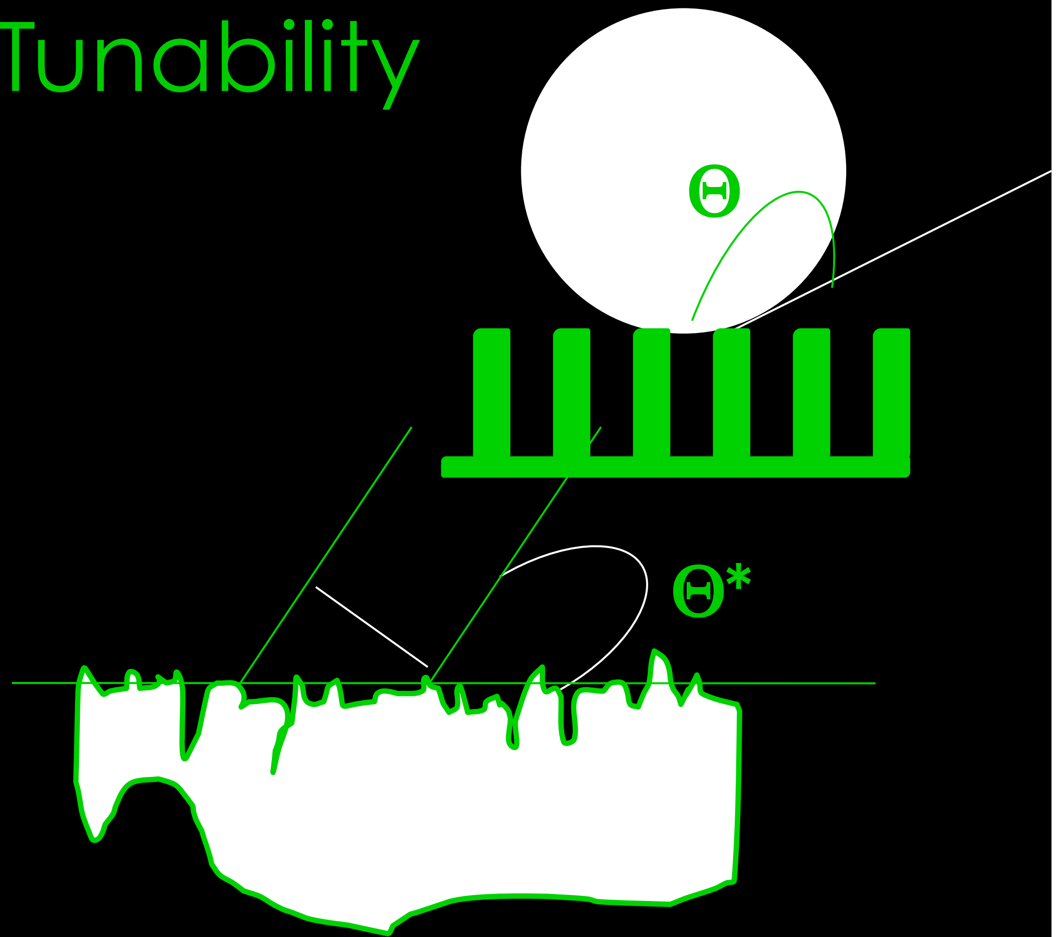


Exemples de lentilles liquides
La fenêtre optique est de 2,3 et 3 mm
www.bulletins-electroniques.com/ti/132_07.htm
Crédits : Varioptic

NANO: LOCALIZATION & CONFINEMENT

–Surface Tension Tunability





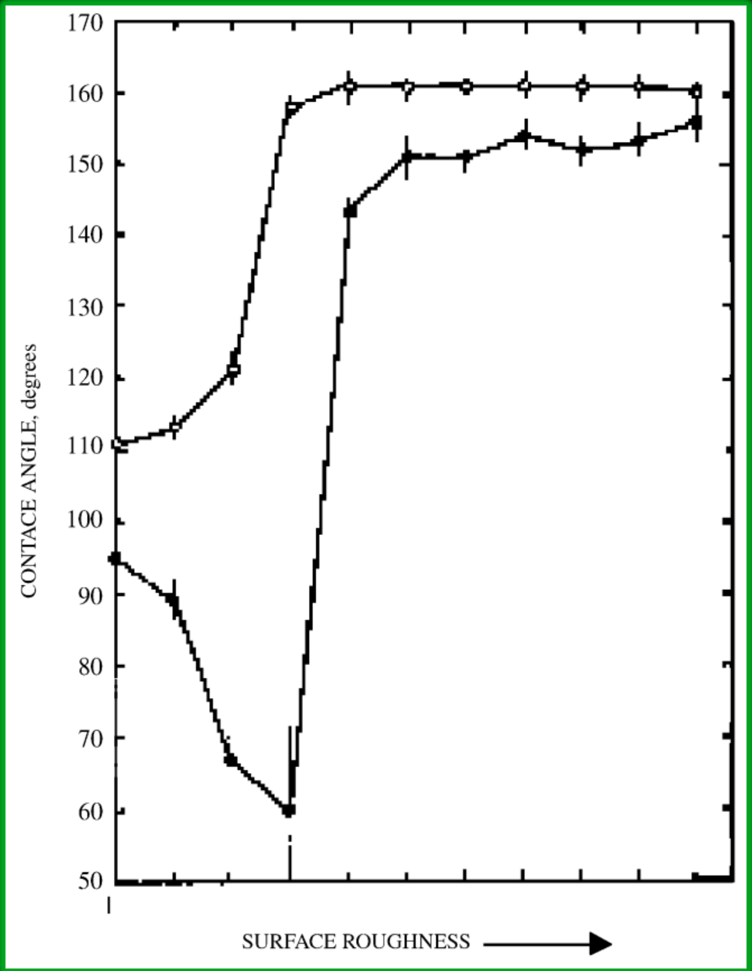
$\cos\Theta^* = f_1 \cos\Theta_1 + f_1 \cos\Theta_2)$

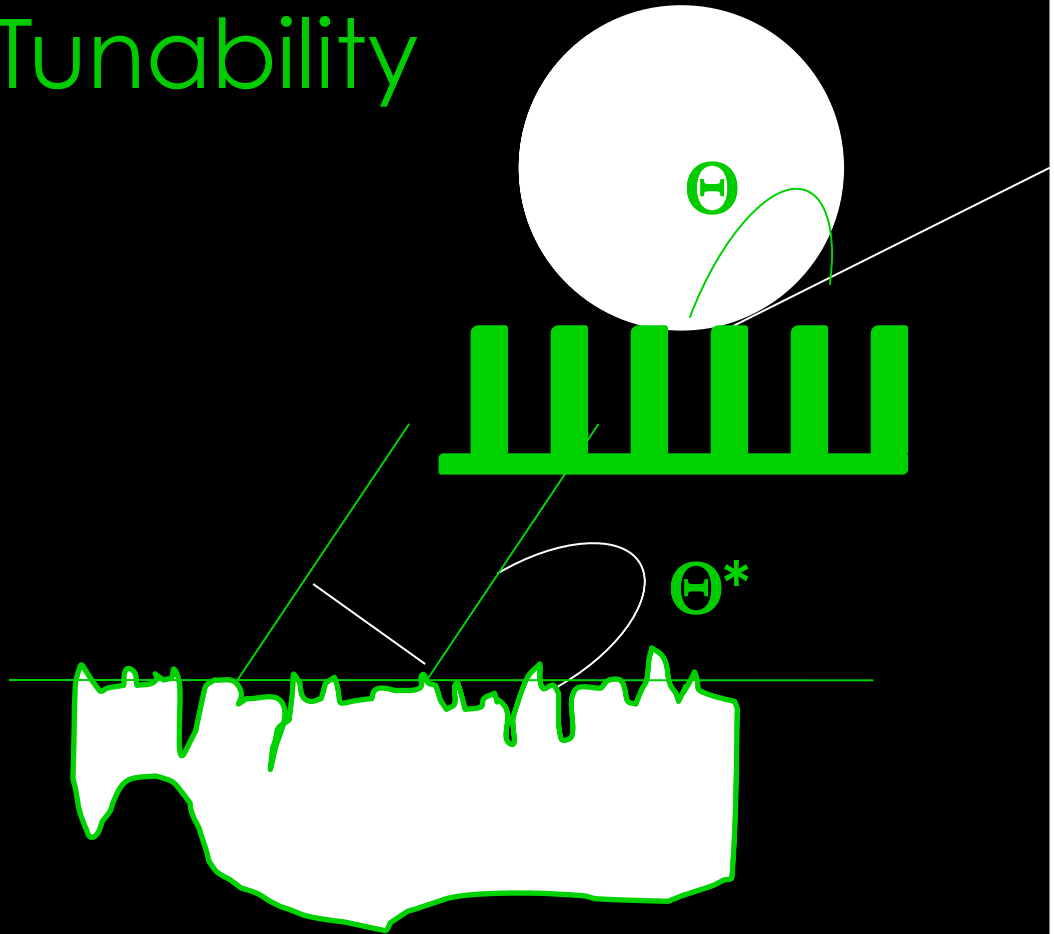
Wenzel/Cassie model

-Wenzel, R.N. Industrial and Engeneering Chemistry, 1936, 28, 988-994.
-Cassie, A.B.D.; Baxter, S. Transactions of the Faraday Society, 1944, 40, 546-551
- Johnson R.E., Dettre R.H., Adv. Chem. Ser.43, 1964, 112-135 [H_2O/ Wax substrates]

NANO: LOCALIZATION & CONFINEMENT

–Surface Tension Tunability





$\cos\Theta^{*} = f_1 \cos\Theta_1 + f_1 \cos\Theta_2)$

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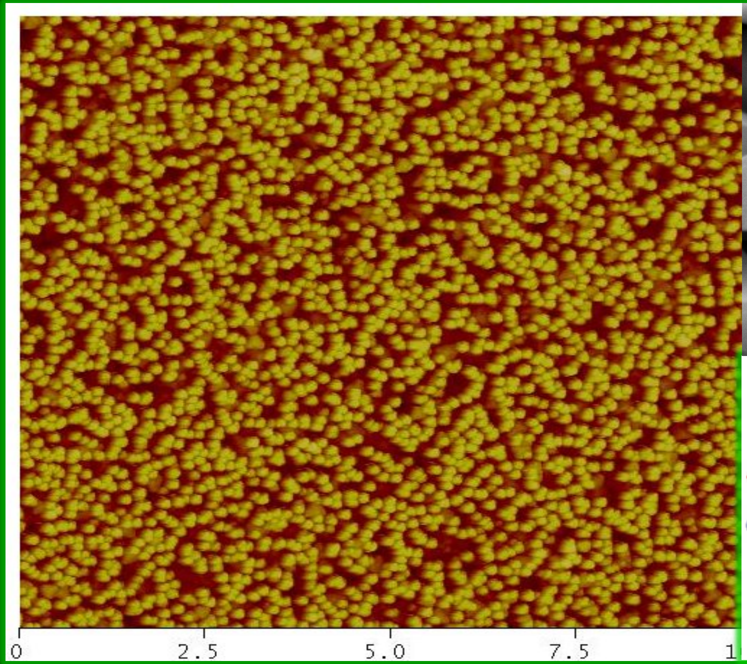
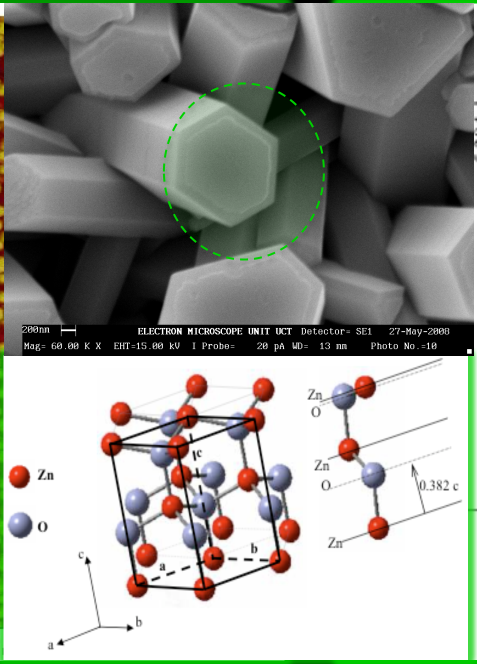
NANO: LOCALIZATION & CONFINEMENT –Surface Tension Tunability

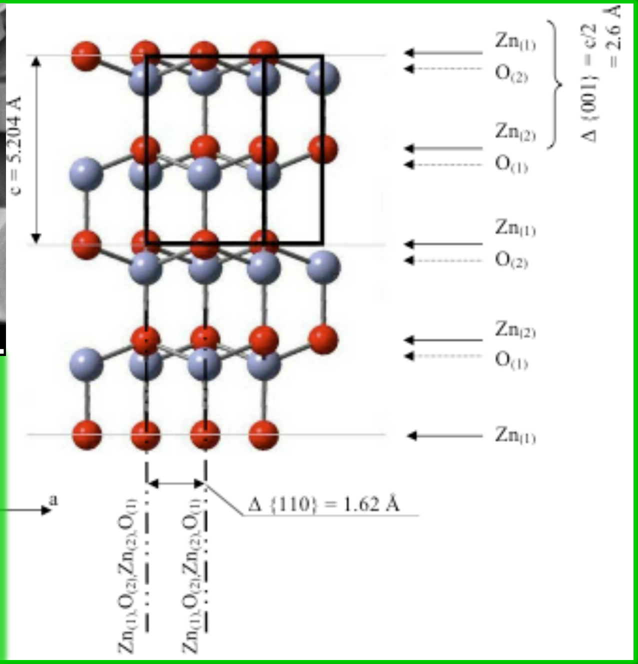
- ZnO: Wurtzite structure
- O-lattice shifted by 0.382 fraction of cell unit heigth "c" from te Zn-latt.
- Reference: Basal Hexagonal plane (001)

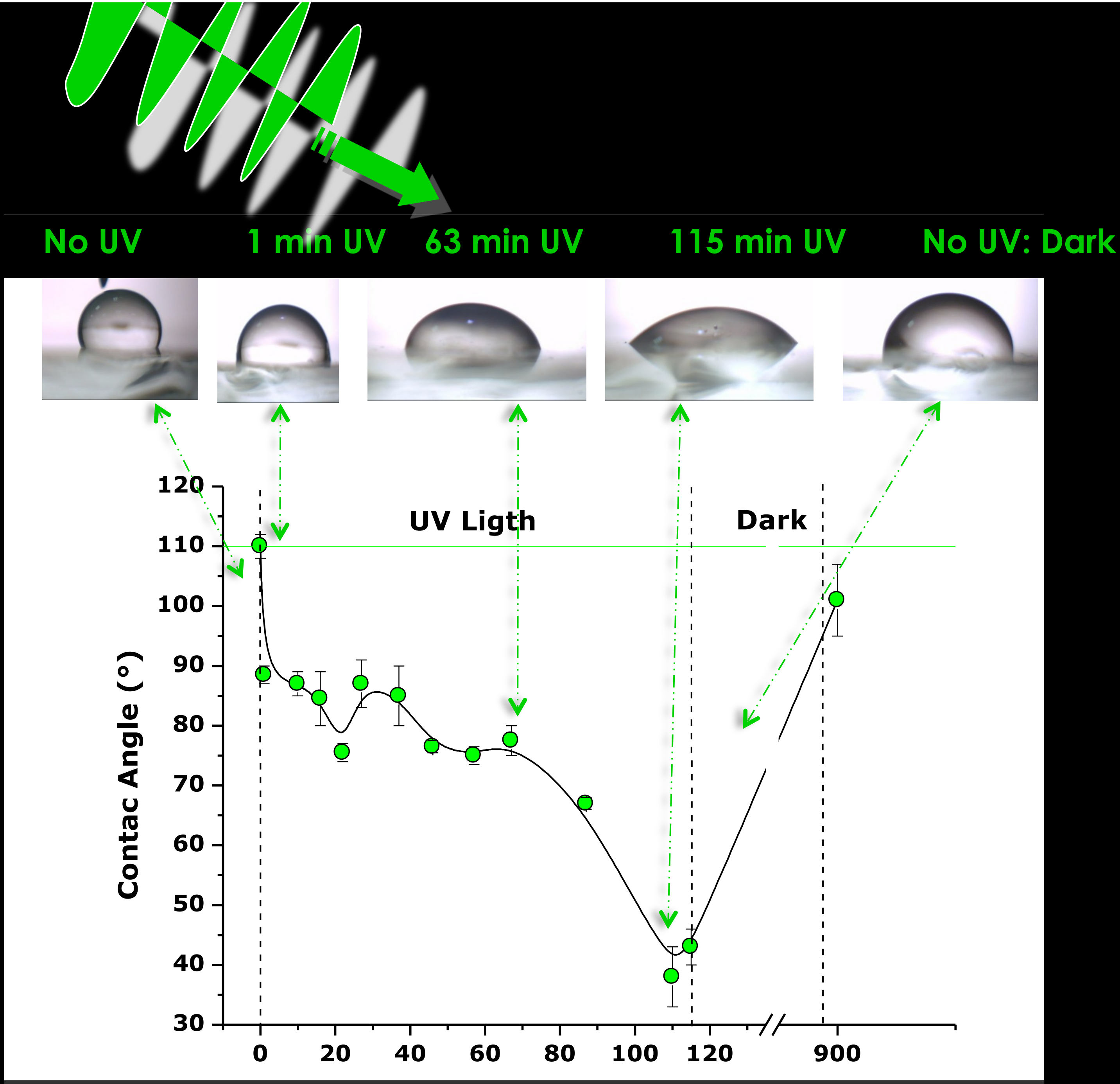
Zn sites: (000) and (2/3, 1/3,1/2)

O sites: (0,0,0.382) and (2/3, 1/3,1/2+0.382)








No UV
1 min UV
63 min UV
115 min UV
No UV: Dark
UV Ligth
Dark
Contac Angle (°)
120
110
100
90
80
70
60
50
40
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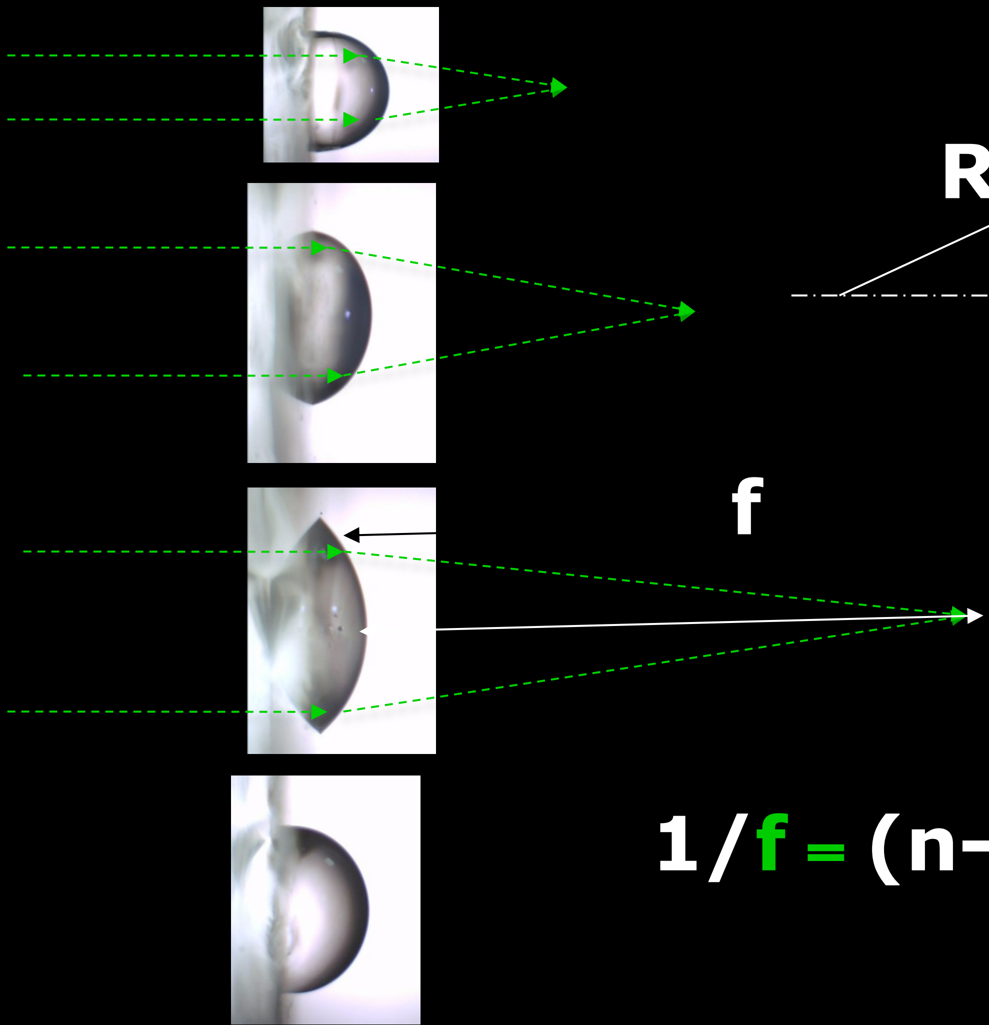
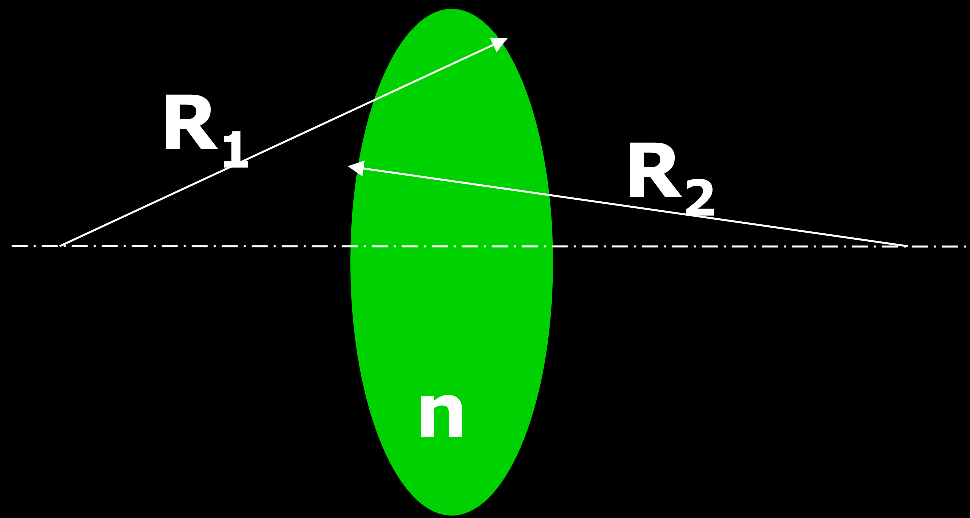
40
60
80
100
120
900

NANO: LOCALIZATION & CONFINEMENT

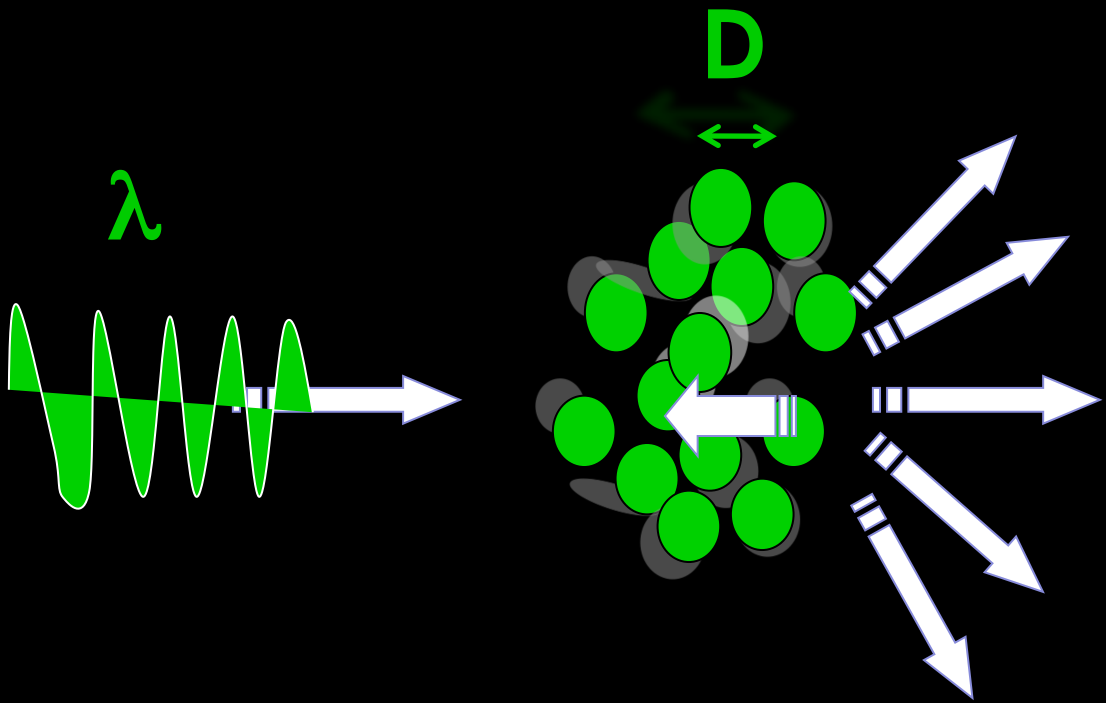
- Liquid lens with tunable focus "f"





$$1/f = (n-1)(1/R_1 - 1/R_2)$$

NANO: LOCALIZATION & CONFINEMENT –Surface Tension Tunability



≠ Scattering cases

•Rayleigh type

$s \;\alpha\; 1/\lambda^4$, $D < \lambda$

•Mie type $D \cong \lambda$, not analytically solvable for arbitrarily shapes

•Anderson loc.: ½ disordered syst. Random walk type

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- Department of Science & Technology of South Africa, Pretoria-South Africa.
- Ministry of Foreign Affairs, Roma-Italy.
- Science & Technology Directorate, French Embassy, Pretoria-South Africa.
- ELETTRA Synchrotron Facility, Trieste-Italy
- African Laser Centre, Pretoria-South Africa.
- African Union-Science & Technology Commission, Addis Ababa-Ethiopia.
- Academy of Sciences for the Developing World, Trieste-Italy.
- Organization of Women in Science for the Developing World, Trieste-Italy.
- International Centre for Science & Technology-UNIDO, Trieste-Italy.
- Centre National pour la Recherche Scientifique, Paris-France.
- The EU-FP7 ICPCNANONET, Brussels-Belgium.
- The National Institute for Materials Sciences NIMS, Tsukuba-Japan.
- Nelson Mandela African University of Science & Technology, Abuja-Nigeria.
- l' Oreal-UNESCO Foundation, Paris-France.
- University of South Africa.
- Islamic Academy of Sciences, Amman-Jordan.

REPVBBLICA ITALIANA

ICTP The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

International Atomic Energy Agency

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THANK YOU, NDIALIVUHA CHUKRAN, MERCI,DANKE

United Nations Educational, Scientific and Cultural Organization

UNESCO-UNISA Africa Chair in Nanosciences/Nanotechnology (South Africa)

UNISA university of south africa

NRF National Research Foundation

iThemba LABS Laboratory for Accelerator Based Sciences