Radioactive Ion Beam and Chemical Perspectives

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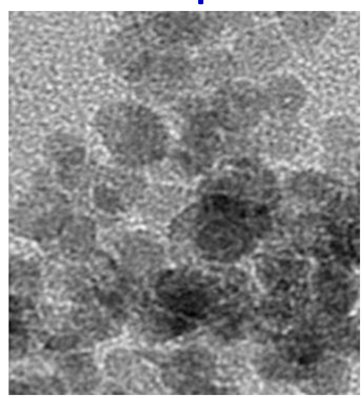
SOLDE Collaboration , CERN

● **Radioactive ion beam** studies in chemistry opens up a new horizon with unlimited scope to alter the **chemical functionality of materials/molecular substances** since the consequences of such interaction remains unknown.

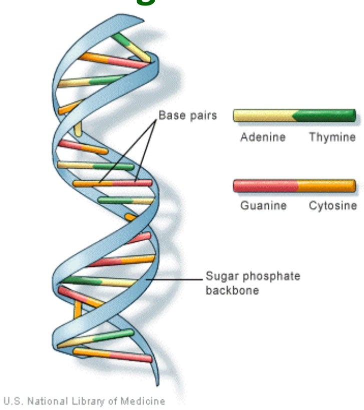
● **Detection of the reactive species** after the exposure to the radioactive ion beam would therefore open up a wonderland in chemical domain.

Here some important domains of work that are focused :

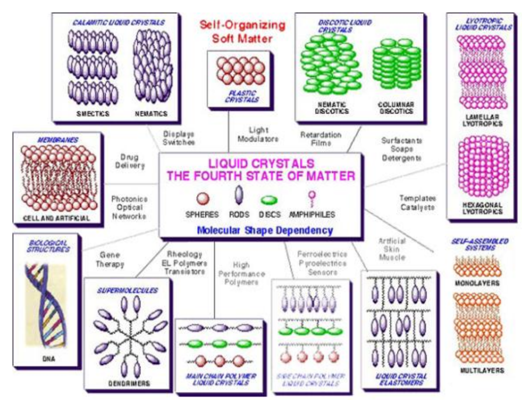
nano size particles



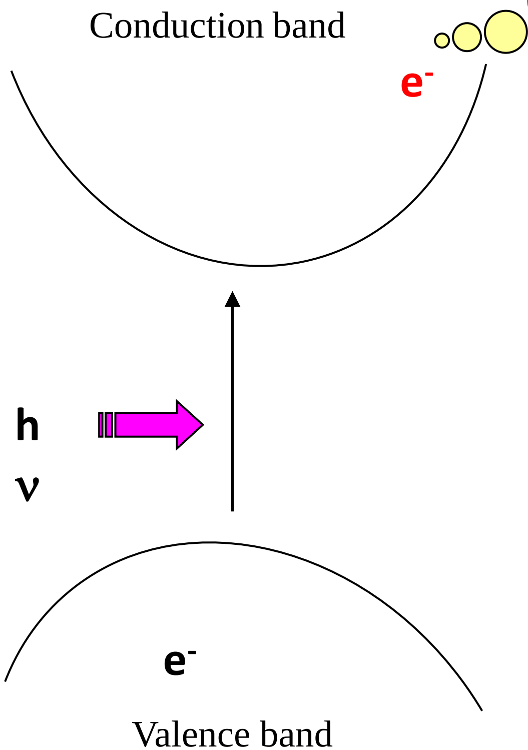
biological molecules

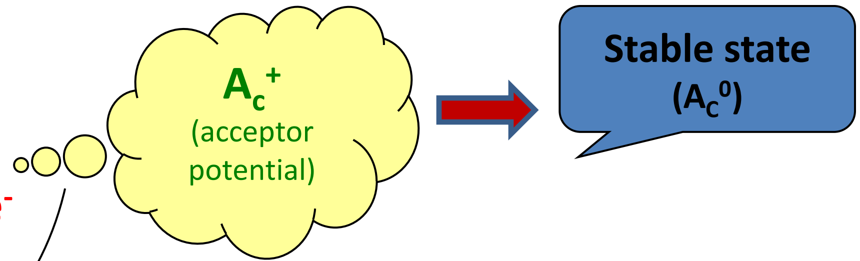


lyotropic liquid crystals



Semiconductor ZnO nano particle





- Nanoparticles are surface active, unusual properties.

- **Optical pumping** of electrons from valence band to conduction band (semiconductor).

- electrons at conduction band is excited at a high reduction potential. If an Ac+ present may take up the e^- charge, **photo induced charge transfer** reactions are important in **biology, device fabrication**

Zinc Oxide nanoparticles grown chemically under the influence of a **biotemplate,** which is Folic acid, for : **size control**, **monodispersity**

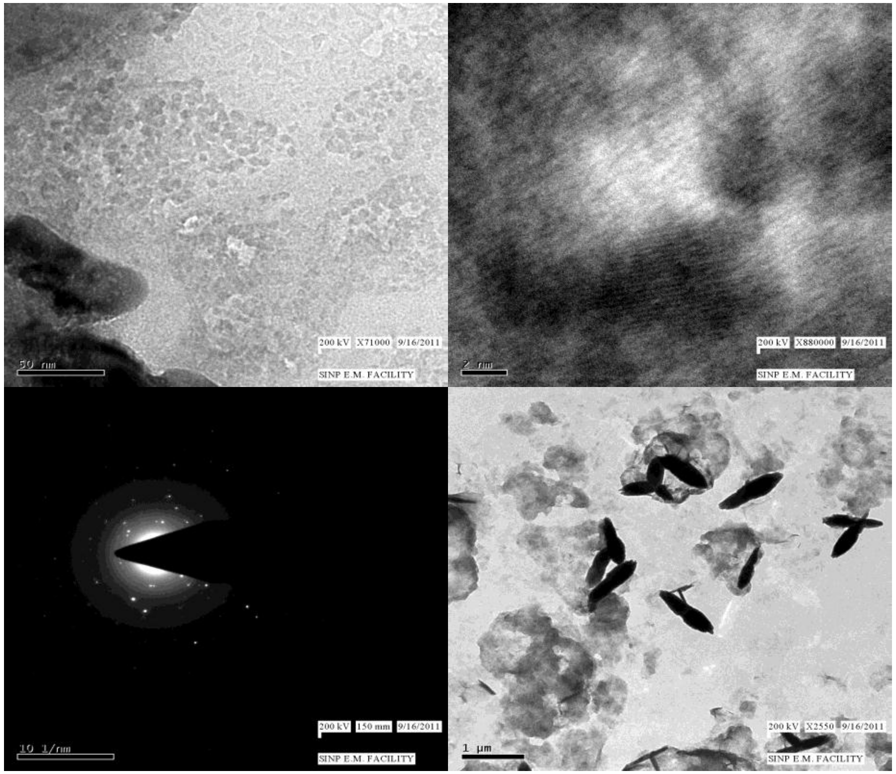
Biotemplate: FOLIC ACID

It regulates the growth of nanoparticles through its charged layer surface properties, prevents **Ostwald ripening**.

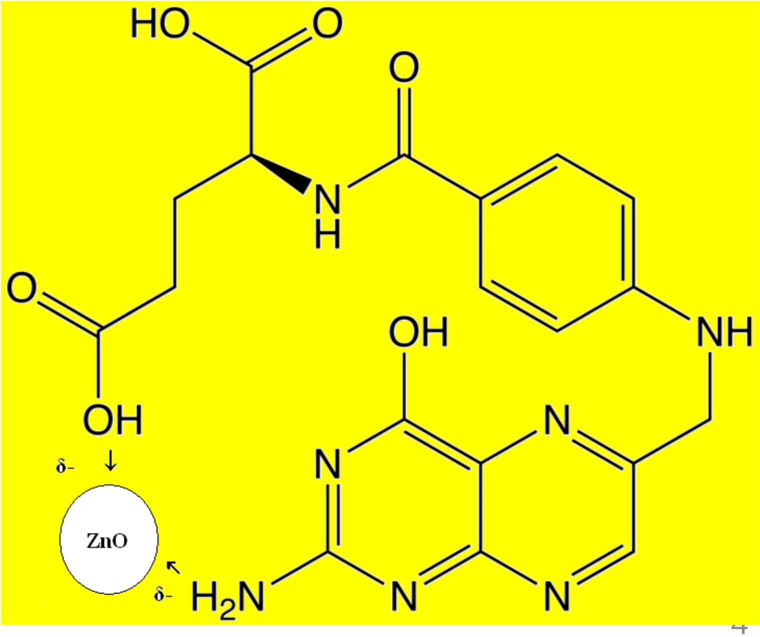
Why we choose Folic acid:

- Folic acid is a member of the Vitamin B family.
- It is necessary for the healthy function of a variety of bodily processes.
- Folic acid is itself not biologically active, but it is biologically important.

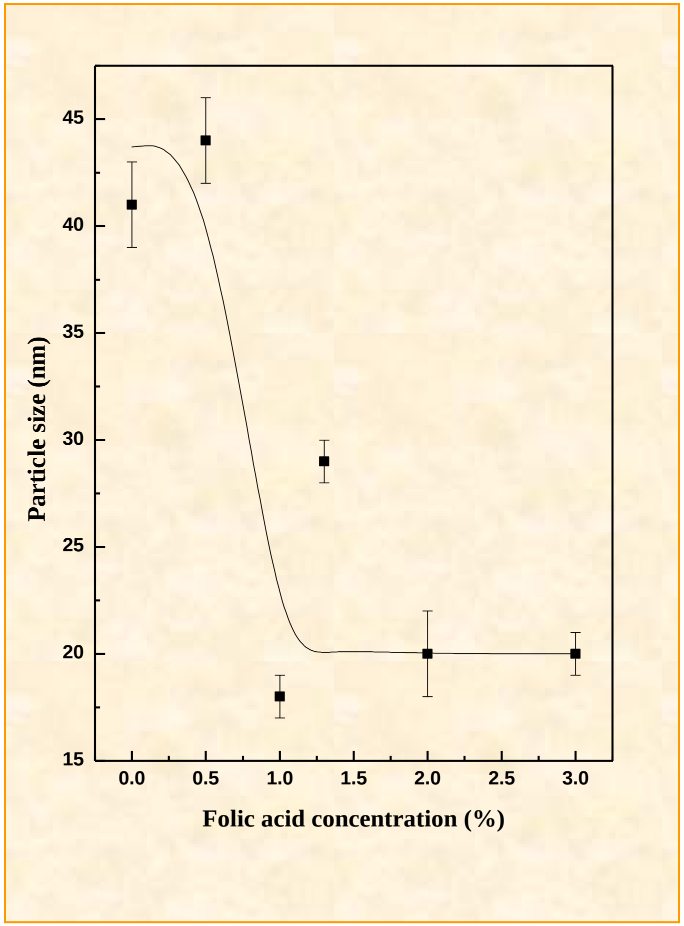
T
E
M



Folic acid ensconced ZnO



Grain Size calculation



Agglomeration no. n = 4/3 (π $r^3\rho$) (N_A/M)

Density of ZnO = 5.606 gm/cm^3

Molecular weight = 81.389 gm/mole

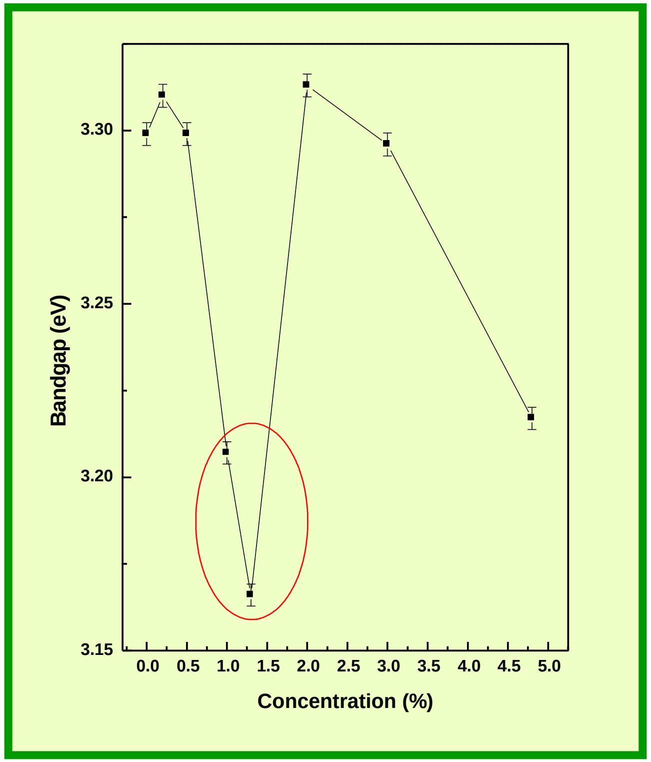
The grain sizes of the powdered samples have been calculated from the Scherrer formula :

$$D_{hkl} = K\lambda/\beta \cos\theta$$

- **The particle size of synthesized ZnO is ~ 41±2 nm.**
- **Particle size decreases (~ 20±1 nm) with increase of folic acid concentration.**
- **In case of 1% folic acid solution, a sharp decrease of grain size (~ 18±1 nm) is observed.**
- **It may be the transition zone.**

Avg. grain size	n	Surface /volume	No. of molecules in the surface
40 nm	$4x10^{24}$	0.1	$4x10^{23}$
20 nm	$2x10^{24}$	0.3	$6x10^{23}$

Ultraviolate-Visible (UV-Vis) Spectroscopy :
Semiconductor Bandgap properties



⇨ The band gap of pure ZnO is ~ 3.3 eV, which is in agreement with the band gap of ZnO prepared by other techniques [Appl. Phys. Lett. 65 (1994) 1373]

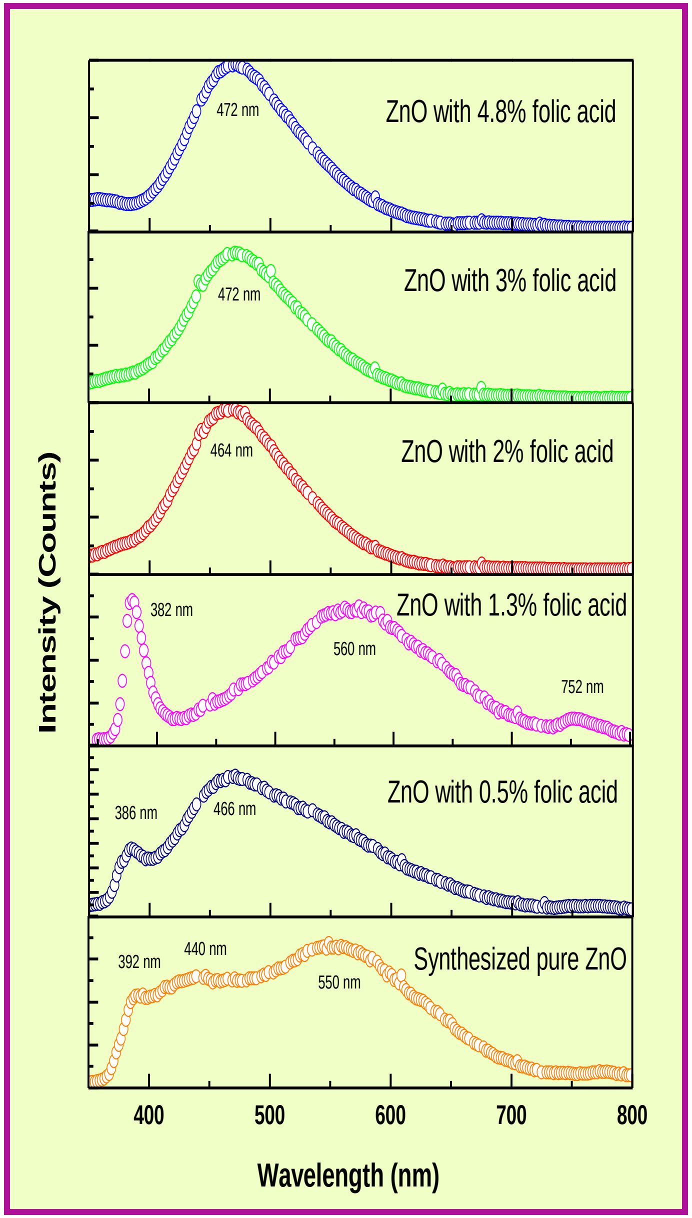
⇨Overall decreasing nature of band gap has been found (from 3.30 eV to 3.22 eV).

⇨ There is so many defect states between the valence band and the conduction band.

⇨ Band gap energy (1% FA solution) = 3.21 eV
Band gap energy (1.3% FA solution) = 3.17 eV

⇓

There is a transition zone in the band gap properties.



⇨**For the as-grown ZnO, there is a broad emission in UV-Visible region.**

⇨ **At 392 nm ⇒ UV emission spectra ⇒ attributed to near band edge emission of ZnO.**

⇨ **With the increase of folic acid concentration (upto 1.3%), UV and visible band are separately distinguished.**

⇨ **With the increase of folic acid conc., the UV emission peak shifts from 392 nm to 382 nm (1.3% conc. of folic acid). It shows a clear evidence of charge transfer reaction.**

⇨ **At 440 nm ⇒ blue emission spectra ⇒ surface defect in ZnO, mainly Zn vacancy.**

⇨ **At 550 nm ⇒ green emission spectra ⇒ excitation from valence band to intra-gap sates.**

⇨**In all samples, green light emission is most prominent.**

⇨**A signature of red emission has been observed in case of 1.3% folic acid concentration.**

⇨ **Above 1.3% conc. of folic acid, only visible emission spectra is prominent.**

USE OF RADIO ACTIVE ION BEAM IN THE ZnO SYSTEM

a) Irradiation with radio active ion beam of $^{67}Cu^{(n+)}$ z=29, $^{68}Ga^{(n+)}$ z=31, $^{111m}Cd^{(n+)}$ z=48 with (Energy range: 10 KV to about 60KV) and appreciable current and fluence needed on the prepared samples.

b) Diffusion of the doped ions (at different oxidation states) : studies can be performed on line (if possible**).**

c) Depending up on doped ionic state and their concentration , spectroscopic properties, **UV-Vis range and PL Studies will be required.**

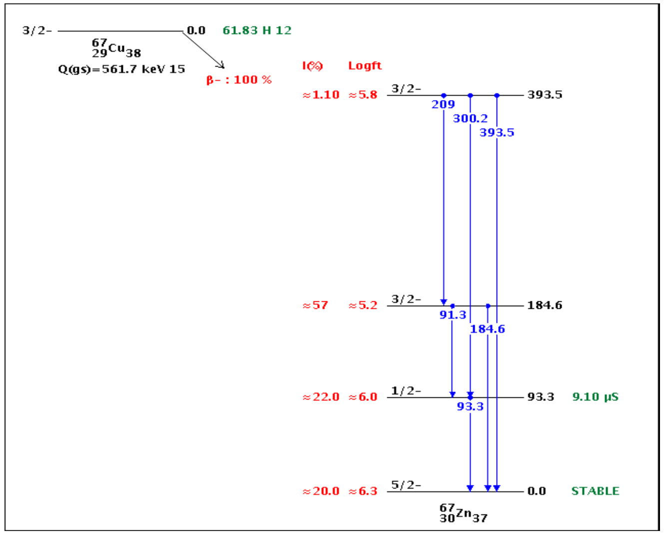
d) Perturbed Angular Correlation (PAC) studies, **with Cd^{111m} is required.**

e) X-ray diffraction data and microscopic studies (SEM/TEM) often needed to examine the irradiation effects for morphological characterization.

f) Positron annihilation spectroscopic studies, at least **Doppler broadening** of the 511 keV line shape can be done (because it is simpler , with ^{68}Ga) and life time analysis can be done either indirectly .or at a later stage.

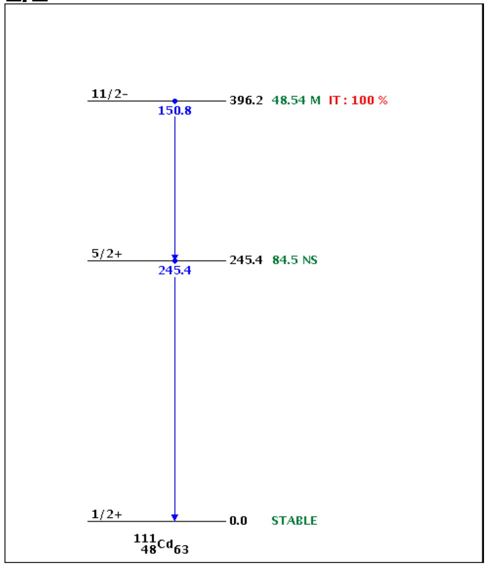
Decay scheme of ^{67}**Cu**$_{29}$

T1/2= 61.83h, β^-

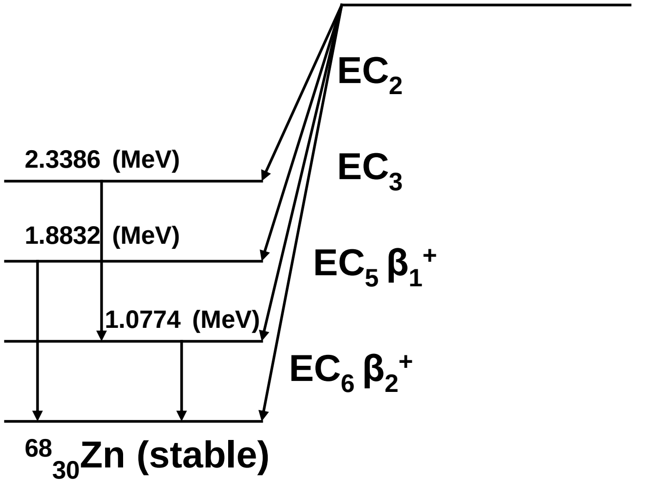


Decay scheme of ^{111}**Cd** $_{48}$, IT

$T_{1/2}$=48.54m



Decay scheme **^{68}Ga$_{31}$, $T_{1/2}$=67.71 m**



Results envisaged :

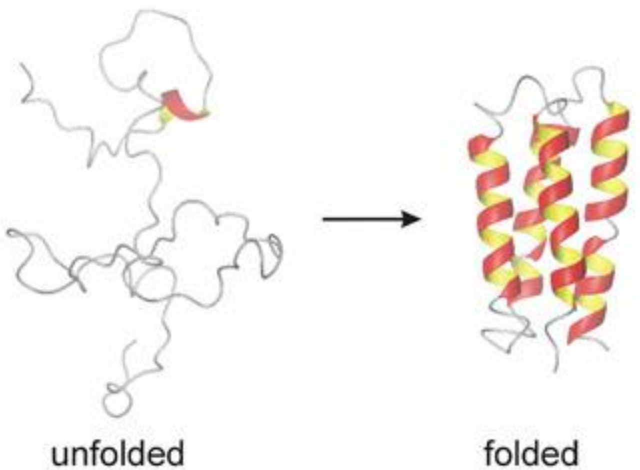
- **Doped ions will bring about a change in crystal structure, create structural defects, induce phase transitions. radiation effects.**
- **Doped material effectively will be a new system with unstable valency state of the radioactive ions, may propagate further changes**
- **Distortion in the lattice due to variation of the ionic radii :** r_{Zn+2}=0.074nm < r_{cd+2} =0.097nm, **there can be lowering of the band gap, important from solar cell point of view (emitting in the visible region)**

Application :

- ZnO is an important nontoxic LED material useful in medicine and biotechnology. The radioactive ion doped and modified material will emerge in a new way in medicine and biology.
- ^{68}Ga is a short lived positron emitter, can be used in connection to PET diagnostics.
- Cu and Ga ions are physiologically active elements, can be useful in nuclear medicine in various ways.

Biological macro molecules

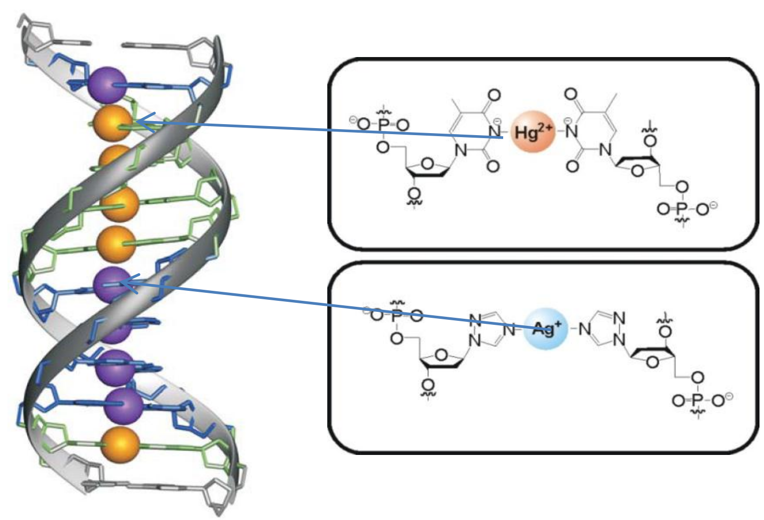
Protein aggregates, **nucleic acid** etc. are some of the important biological macro molecules which could host metal ions when doped in regulated quantities. It could have wide implication in their functionalities. An energy dependent doping of metal ions as micro nutrients in biological systems could be meaningfully utilized towards their medicinal usage.



Metal ion binding to proteins may lead to a special functional form, eg.

Azurin – an example of a Cu(I)/Cu(II) dependent electron transporting protein

• **binding sites in biomolecules**



Metal-mediated base pairs represent a powerful tool for the site-specific functionalization of nucleic acids with metal ions. Nature Chemistry 2, p 229–234(2010)

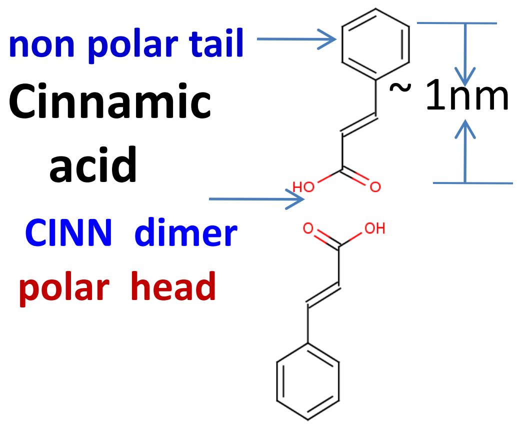
Lyotropic liquid crystals

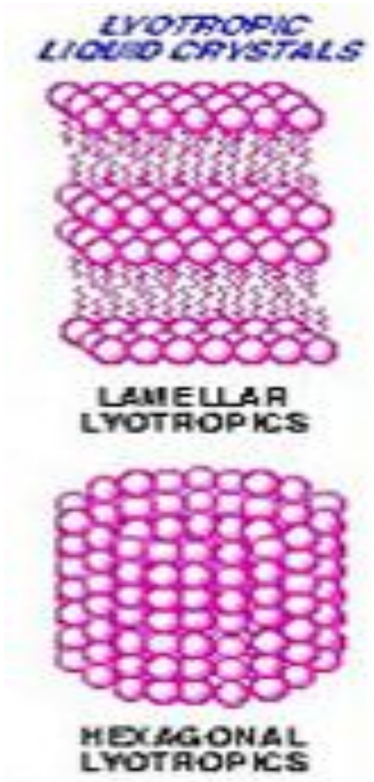
lattice constants range from several nanometers to tens of nanometers, perfect template candidate for designing novel materials by doping with radioactive ion beam,

- different energy scale and low current conditions
- study the properties of the structural modifications.

CINN exerts its antiproliferative effcts by inhibition of protein isoprenylation:

- the protein **'cysteine'** has a terminal **'thiol (-SH) group'** at its residue.





#if CINN gets the (-SH) moiety it stacks up subsequently
- this results in differentiation/blocking the pathway for cell division - thus tumour growth is prevented !

forms a <u>crystalline layered structure</u> also in solid state - PAS can be helpful to elucidate structural aspects
bulk **PAS studies (LT, DB)** revealed a heterogeneous layer structure for CINN crystalline grains [6]
we try to probe the stacking feature (supra-structure) of CINN deposited on different substrates

summary

Modification of substrates and their detection/ structural identification

- Nano size semi conductor particle
- Bio macro molecules
- Lyotropic liquid crystals

Thank you
& Looking forward
to collaboration