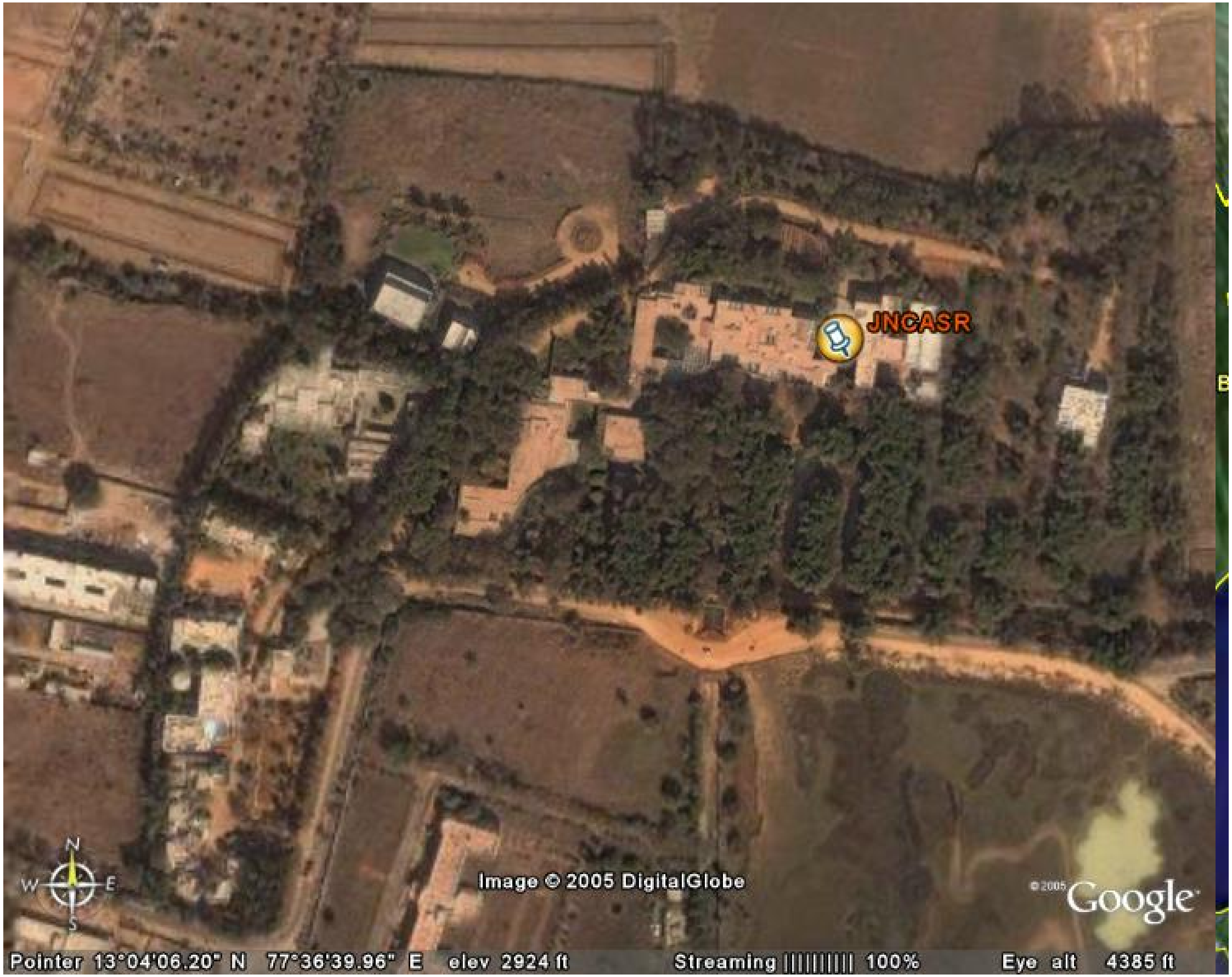
Materials Research at JNCASR Bangalore India

K.S. Narayan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JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH

An autonomous institution of Department of Science and Technology, established in 1989

CHARTER

- To carry out front-line research in selected thrust areas of science and engineering;
- To promote collaborative research with scientists at the Indian Institute of Science and other institutions in the country;
- To provide a national and international forum for in-depth discussions on important scientific topics in areas of vital interest to scientists of the Centre and in the country at large;
- To organize periodic winter and summer schools in certain areas, where young talented scholars would be associated;
- To provide opportunities for talented young students to carry out research projects;
- To provide facilities to visiting scholars and faculty from all over India and abroad, to work for extended periods with the faculty of the Centre;
- To publish monographs and reports on frontier and futuristic areas of science as well as monographs of educational value.

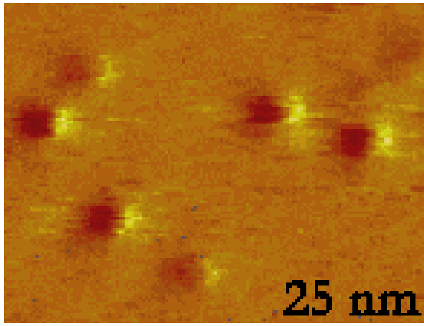
Academic Activities

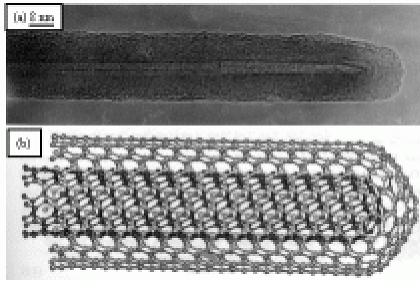
- Chemistry and Physics of Materials
- Evolutionary and Organismal Biology
- Molecular Biology and Genetics
- Theoretical Science
- Engineering Mechanics
- Geodynamics
- Education Technology

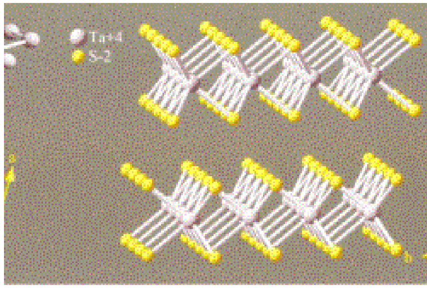
Chemistry and Physics of Materials Unit

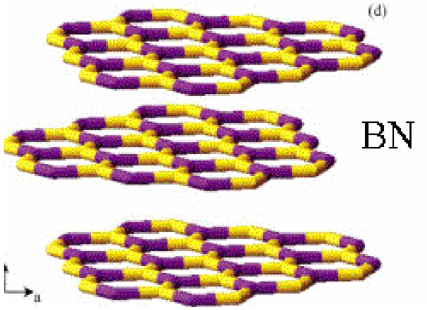
Chair: Prof. C.N.R. Rao

Faculty: Prof. K.S. Narayan, Prof. G.U. Kulkarni, Prof. S. Balasubramanian, Dr. Easwaramurthy, Prof. Chandrabhas Narayana, Dr. A. Sundaresan









- **Core theme:** Studies of novel and functional materials.

- Experimental and computational approaches are employed to understand physical and chemical phenomena, at the atomic and molecular level.

- **Research Areas:**
  - Synthesis, structural, electrical, and magnetic properties of nanomaterials, Nanocomposites, nanolithography cluster beams, interfaces, colossal magnetoresistive oxides, thin films, gas sensors, and novel mesoporous materials.
  - Molecular electronics using conducting polymers, devices and biophotonics.
  - Optical spectroscopy of materials under extreme conditions.
  Molecular simulations of green solvents, materials, and protein solutions.

- **State-of-the-art facilities:**
  - Floating zone furnace, atomic force, scanning tunneling microscopes, transmission and scanning electron microscopes, high-speed optoelectronic lab, diamond anvil cell to attain pressures up to 30 GPa, 15 Tesla superconducting magnet, single crystal and powder x-ray diffractometers, IR-vis, Raman and Brillouin spectrometers, and Beowulf parallel computers

Theoretical Sciences Unit

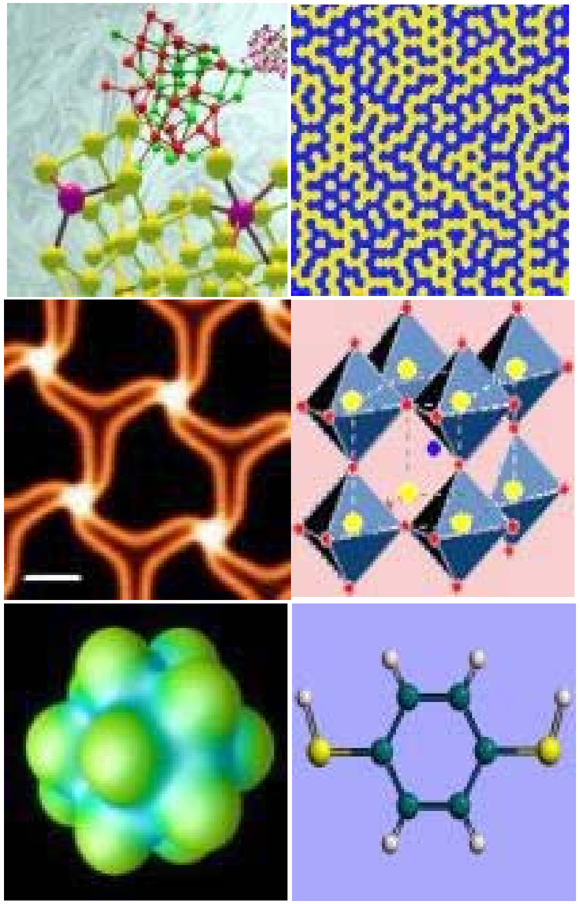
JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH

Chair: Prof. Rahul Pandit

Faculty: Prof. Shobhana Narasimhan, Prof. Srikanth Sastry, Dr. Umesh V Waghmare, Dr. Swapan K Pati, Dr. Vidhyadiraja

- Study of a range of materials and phenomena of fundamental and technological interest using theoretical methods including state-of-the-art computation.

- Glass-forming liquids, water, silicon, organic molecules, conjugated polymers, inorganic solids, simple, noble and transition metals and their surfaces, ferroelectrics, complex insulators close to metallicity, nanoclusters, magnetic semiconductors, and biomolecules.



Molecular Biology and Genetics Unit

The Theme

Application of biotechnology to study and control disease

- **Malaria**
  - Study of parasite enzyme pathaways
  - Structure determination of parasite enzymes
  - Developing anti-malarial drugs Triclosan
  - Screening natural compounds with anti-malarial activity
- **DNA Organization**
  - How DNA is reorganized when sperms are formed
  - How failure in DNA damage repair leads to cancer
  - How gene expression from human genes is controlled
  - Searching for natural products with anti-cancer properties
- **Blood vessel formation**
  - How blood and blood vessels form in normal and cancer cells
  - Knowledge useful to control tumors
  - Use of embryonic stem cells transgenic mice, Drosophila genetics
- **Human genetics**
  - Study and search for genes involved in genetic disorders Epilepsy, Deafness, Speech disorders
- **HIV/AIDS**
  - Identification of viral subtypes in India
  - Study of Indian viruses: Pathogenesis, Molecular biology
  - Engineering genetic vaccines for HIV
  - Developing diagnostic tests for HIV

Engineering Mechanics Unit

Chair: Prof. R. Narasimha

Faculty: Dr. Meheboob Alam
Prof. Rama Govindarajan
Dr. Sreenivas K. R.

- **Major areas and their applications:**
  - Understanding clouds, monsoon rainfall (weather models)
  - Insect flight (micro-air vehicles)
  - Turbulent flow control (drag reduction)
  - Near ground temperature distribution (agriculture meteorology)
  - Nano mechanics, granular flows (avalanches & mud slides)

EVOLUTIONARY AND ORGANISMAL BIOLOGY UNIT

Chair : Prof M K Chandrashekaran
Faculty : Prof Amitabh Joshi, Dr Vijay K Sharma
Distinguished Fellow : Prof Gerhard Neuweiler
Hon. Professors: Prof Raghavendra Gadagkar, Prof Vidyanand Nanjundiah

- **The only research outfit in India investigating a variety of ecological, physiological and evolutionary problems.**

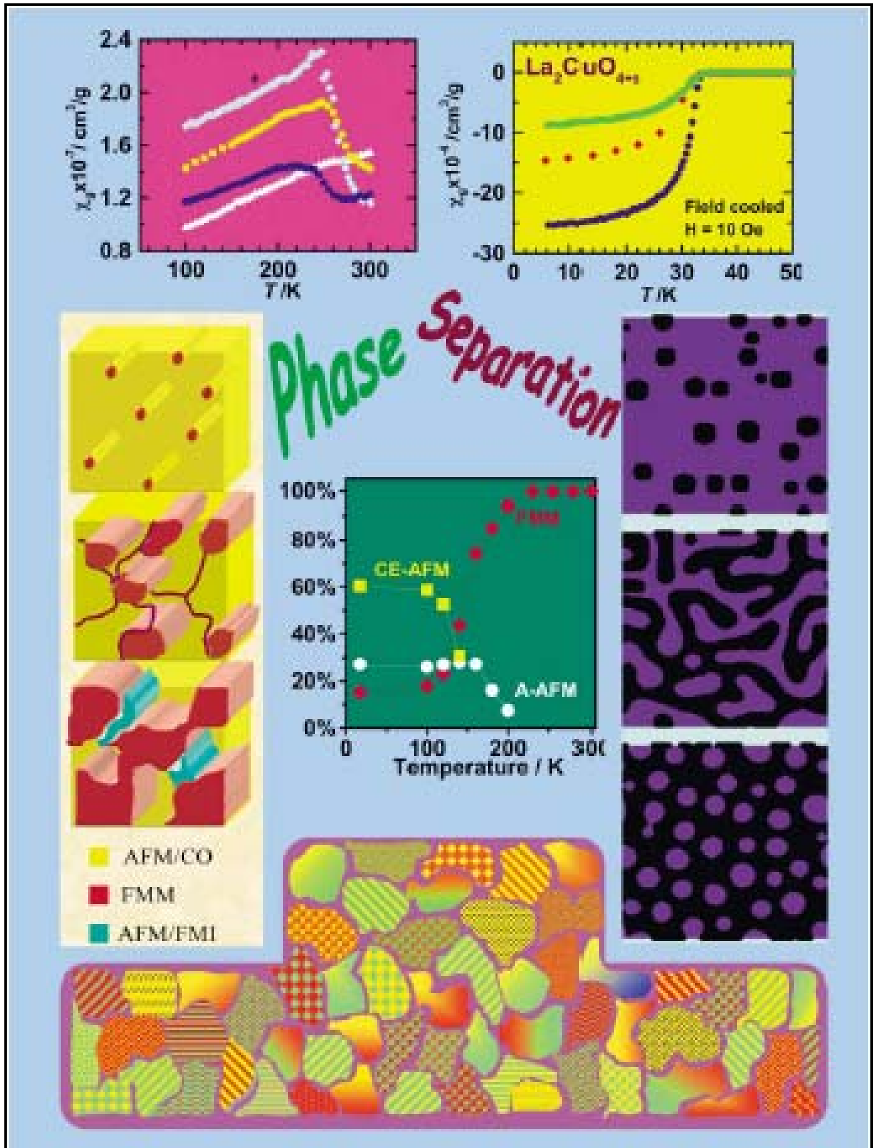
- **Thrust areas include**
  - **Chronobiology : biology of time keeping**
  - **Evolutionary biology**
  - **Behavioural ecology and sociobiology.**

- **Significant contributions :**
  - **Circadian clocks by fruit fly raised in an aperiodic regime shown to be functional for seven hundred generations**
  - **Multioscillatory architecture of circadian clocks elucidated in fruit fly**
  - **Effect of aging on the circadian clocks of mice**
  - **Circadian consequences to the social organization of ant colonies.**

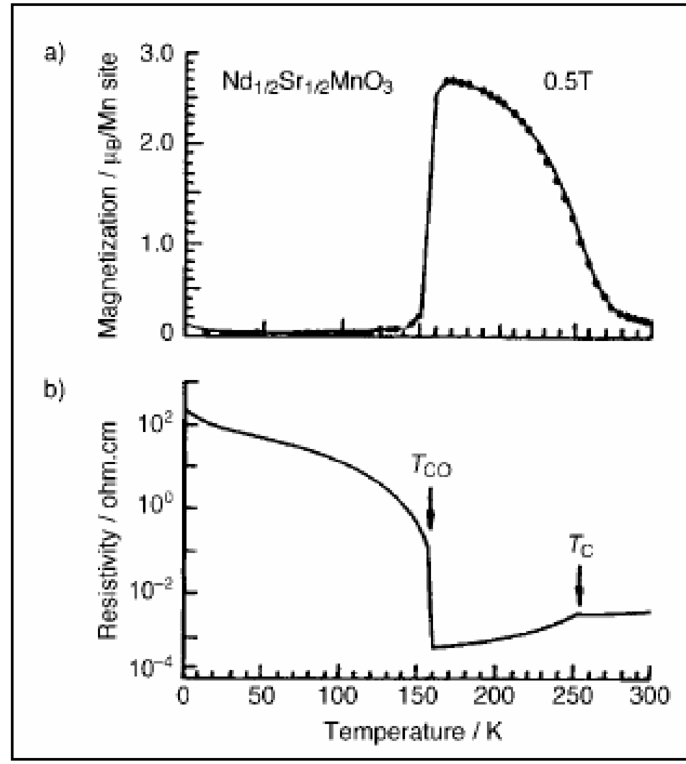
- Materials Physics and Chemistry (Experimental and Theory)

- # of Refereed International Publications in 2004 ~ 110
- # of Refereed International Publications in 2005 ~ 125

Prof. C.N.R. Rao's group - Transition metal oxides



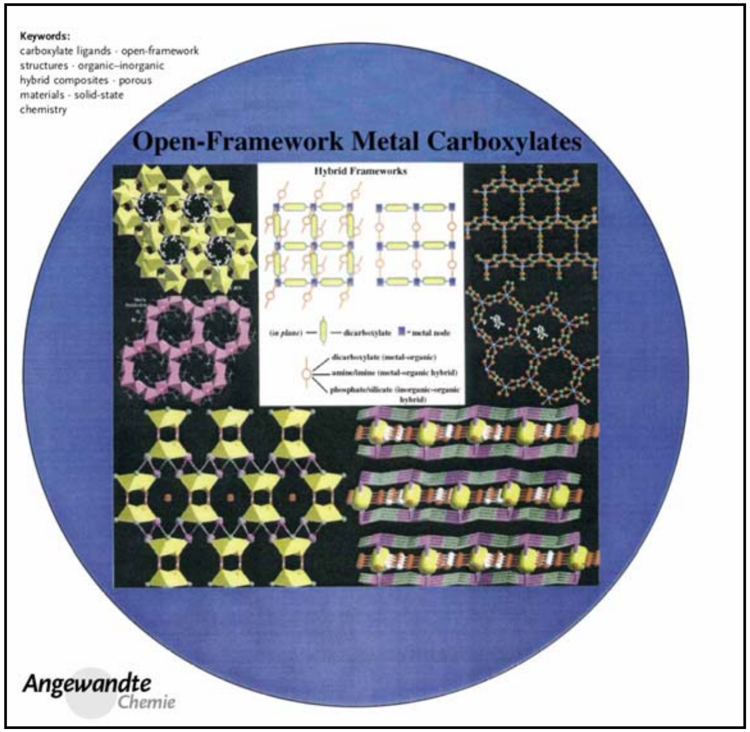
Phase separation in transition metal oxides



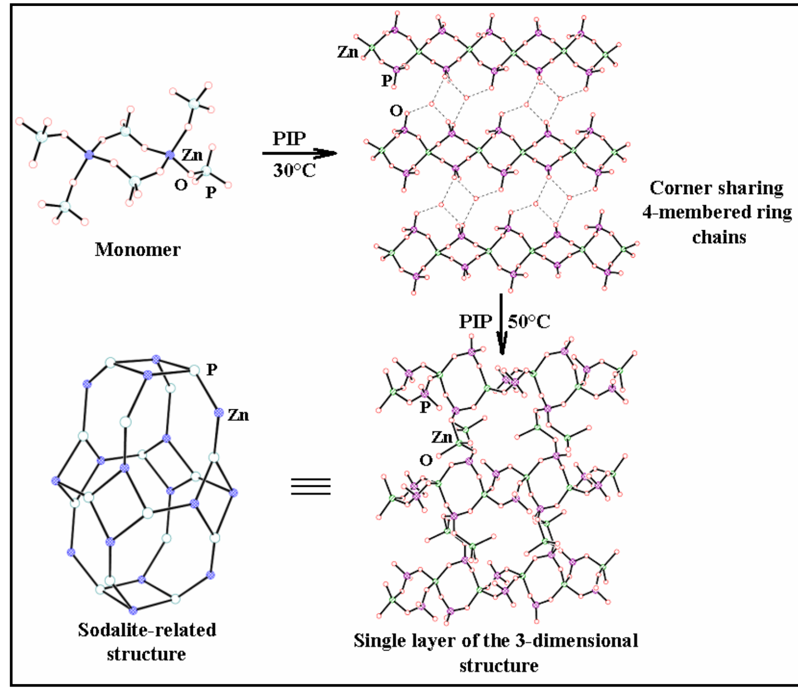
Temperature variation of a) magnetization and b) resistivity of $Nd_{0.5}Sr_{0.5}MnO_3$

For References visit:
http://www.jncasr.ac.in/cnrrao

Open Framework Materials



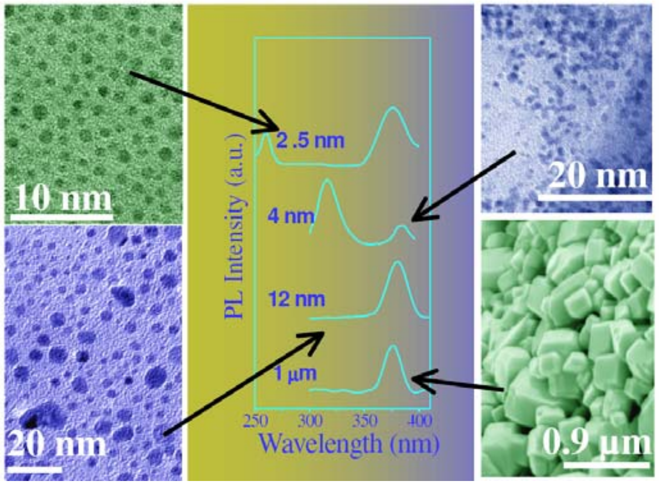
Various metal carboxylate frameworks



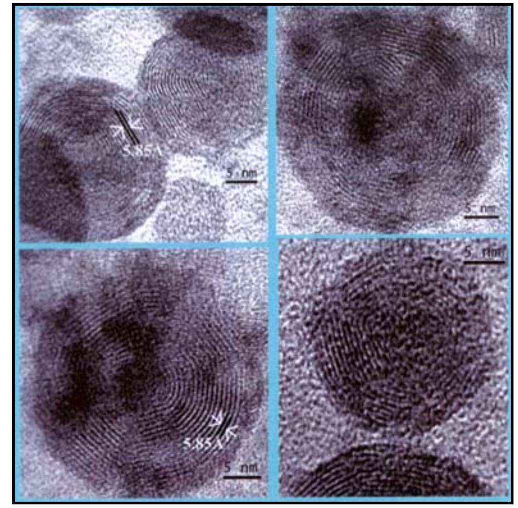
Transformation based on reaction conditions

Nanomaterials – Nanoparticles and Inorganic Fullerenes

Synthesis:

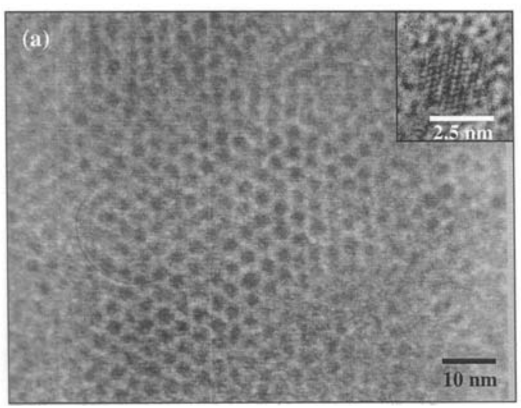


Gallium Nitride

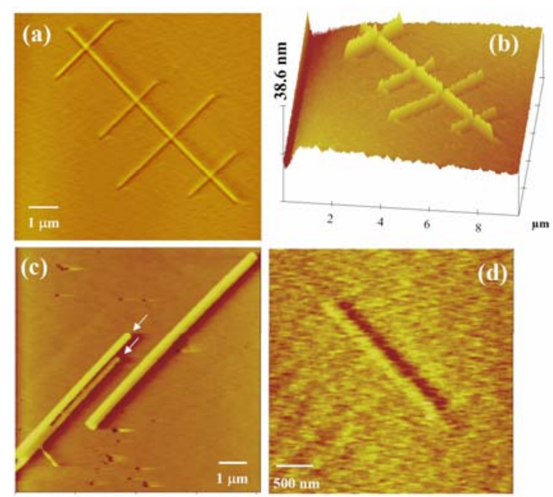


Hf_2S fullerenes

Assembly of nanoparticles:



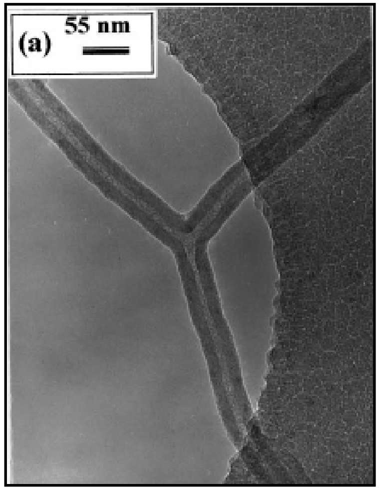
Self-assembly- Pd_{561}



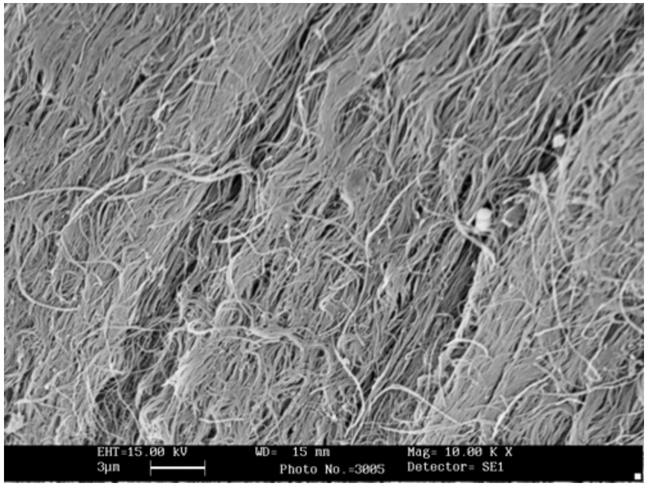
Dip pen lithography with γ-Fe_2O_3

Nanomaterials – Nanotubes and Nanowires

Carbon Nanotubes

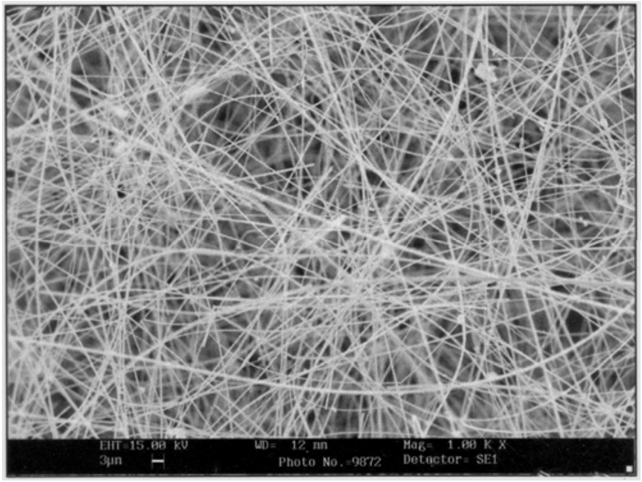


Y-junction

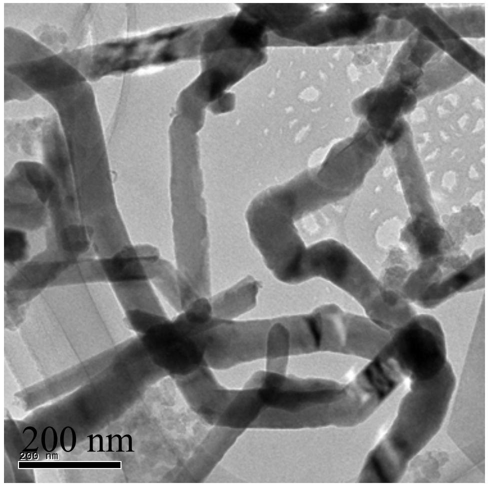


Aligned MWNT bundles

Nanowires



Silicon nitride

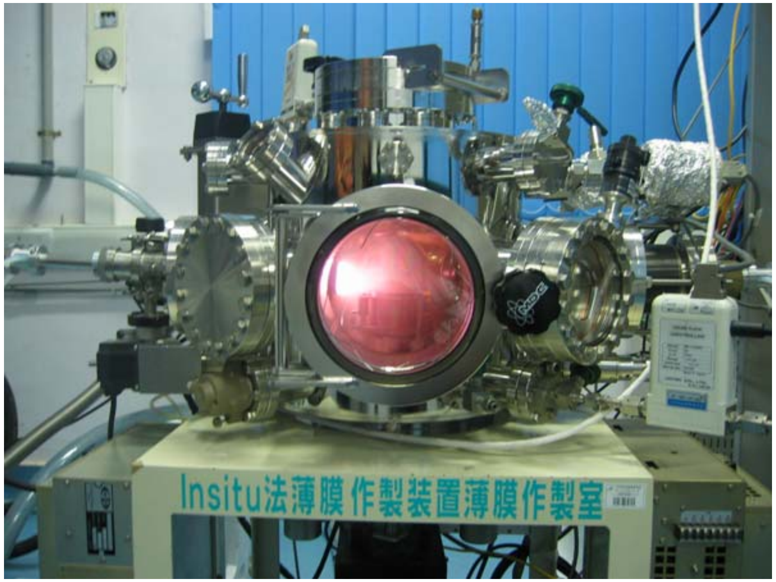


Zinc

Preparation and study of novel functional oxides

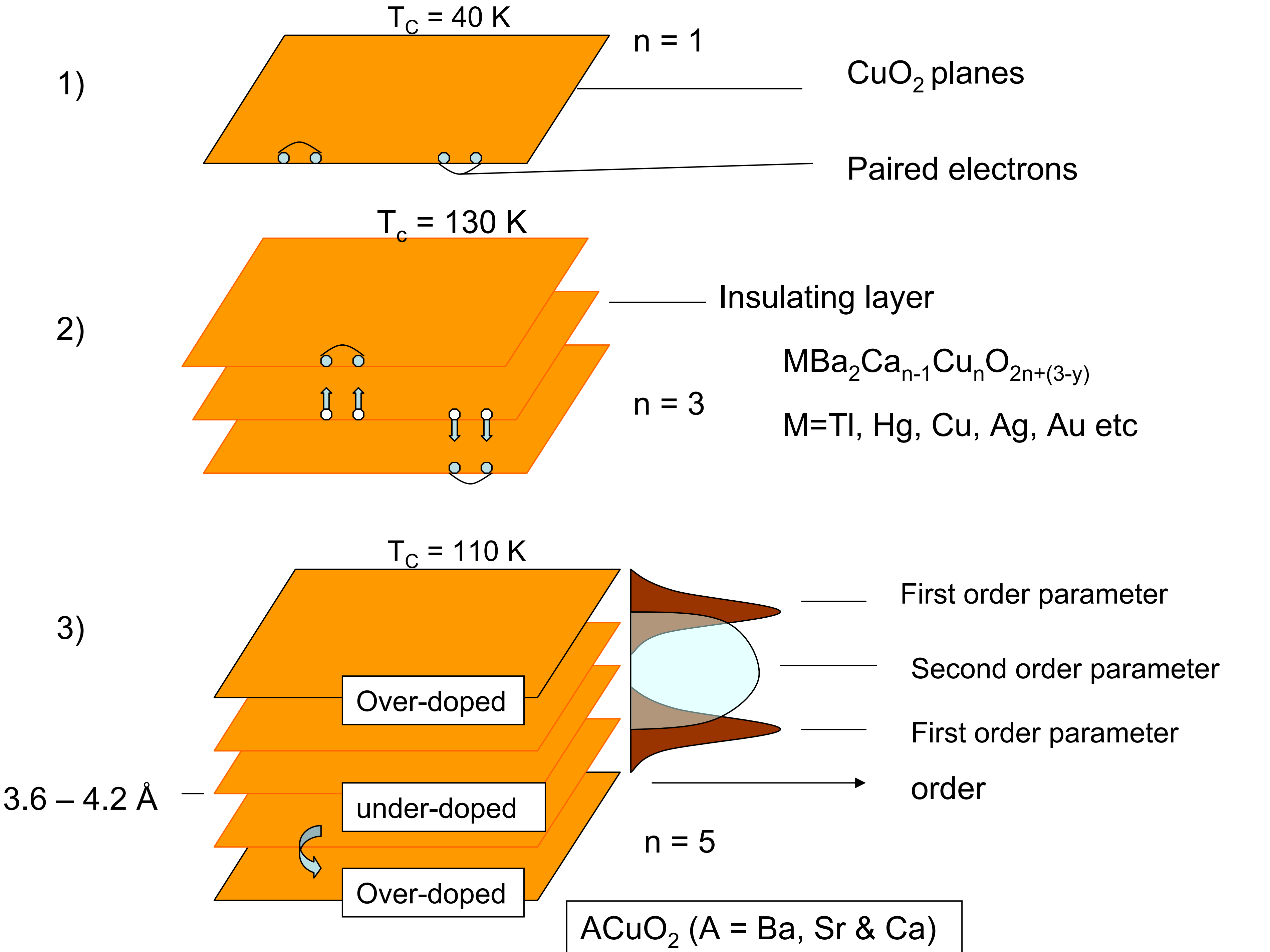
- Preparation of new materials with novel electrical and magnetic properties including multiferroic materials and improve their properties by studying the relationship between the structure-properties.
- Fabrication of superlattices of High Tc cuprate superconductors and ferromagnetic layers. These materials will be achieved by using RF magnetron sputtering method which can control the growth in the atomic scale.
- Atomic engineering by layer-by-layer deposition of $ACuO_2$ (A = Ba, Sr, & Ca) layers on suitably lattice matched substrates

Ever cool PPMS (9 T) with VSM, ac-χ, heat capacity and AC-transport options



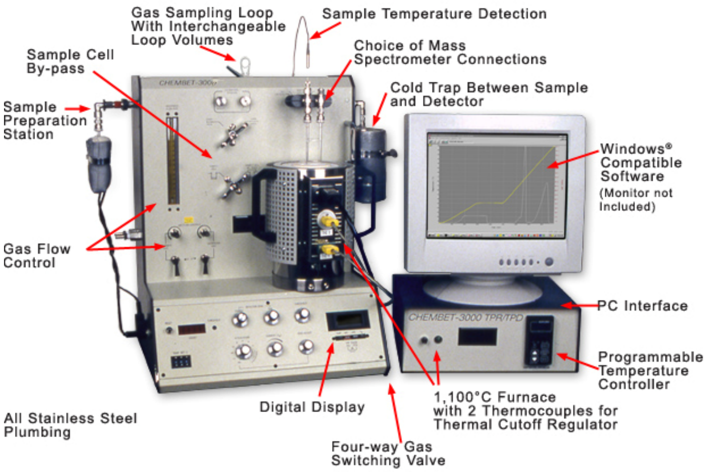
Computer controlled multitarget RF magnetron sputtering machine for the growth of superlattices

Precision Workstation (Radiant Technologies) for dielectric test measurements



1)
T_C = 40 K
n = 1
CuO_2 planes
Paired electrons
2)
T_c = 130 K
Insulating layer
$MBa_2Ca_{n-1}Cu_nO_{2n+(3-y)}$
M=Tl, Hg, Cu, Ag, Au etc
n = 3
3)
T_C = 110 K
First order parameter
Second order parameter
First order parameter
order
Over-doped
under-doped
Over-doped
3.6 – 4.2 Å
n = 5
$ACuO_2$ (A = Ba, Sr & Ca)

Adsorption system



Particle size and Zeta potential analyzer

1. To measure the Surface area, Pore size distribution, Acidity and Basicity of nanoparticles and mesostructured materials.

2. To study the H_2, O_2, CO and CO_2 chemisorption as well as the adsorption behaviour of organic vapours on nanoparticles, nanotubes and mesostructured materials .

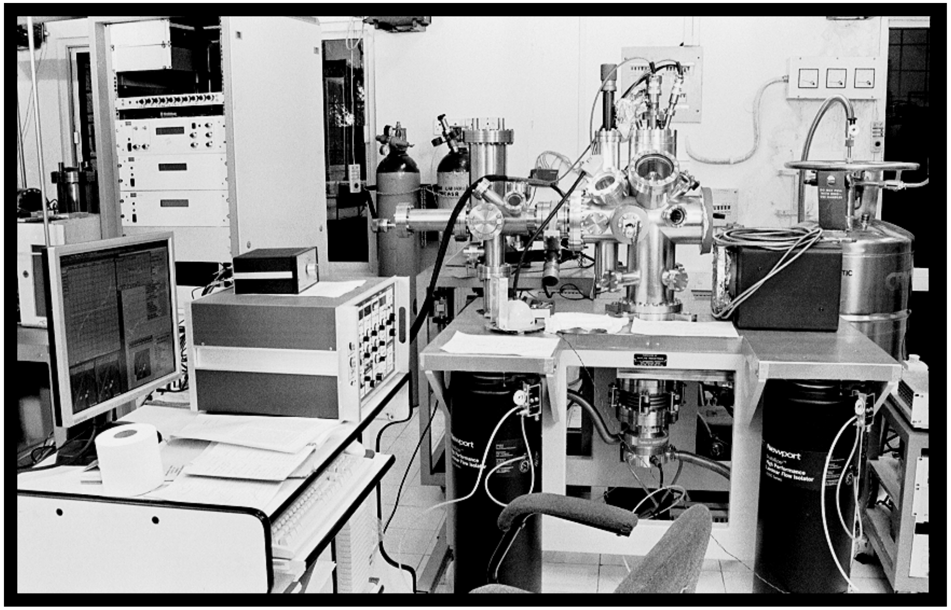
Measure the particle size ranging from 0.6 nm - 6µm

& Zeta potential between 3nm - 10µm and

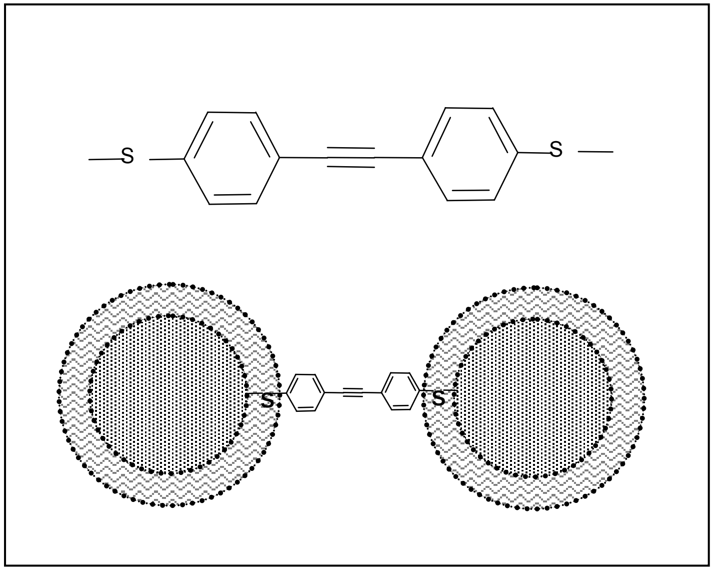
Molecular weight measurement between 1×10^3 Da and 2×10^7 Da

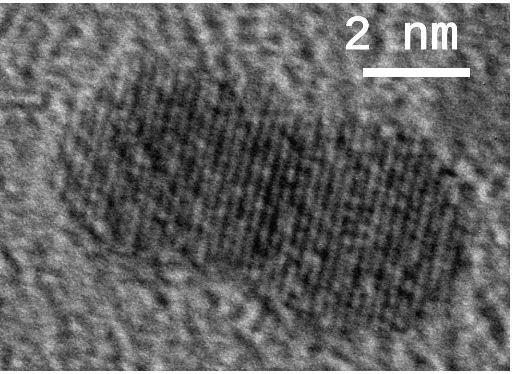
• Low temperature scanning tunneling microscope

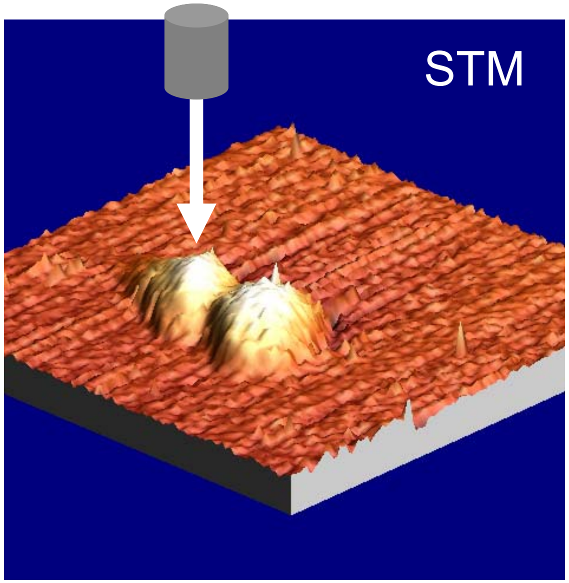
GUK-1

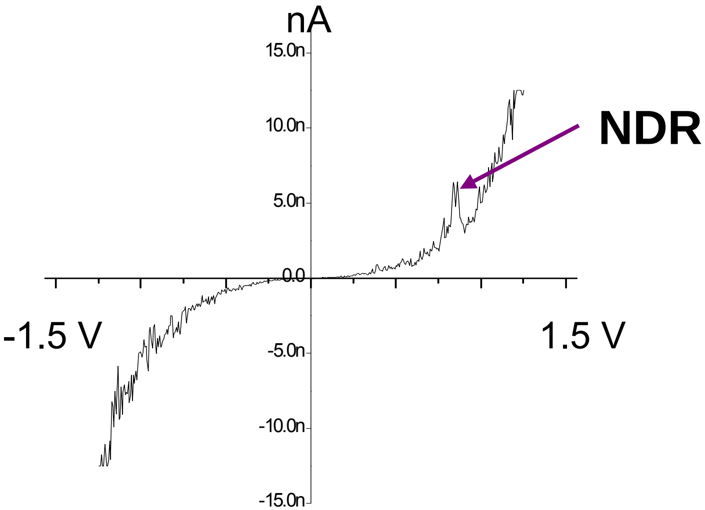


A molecular switch





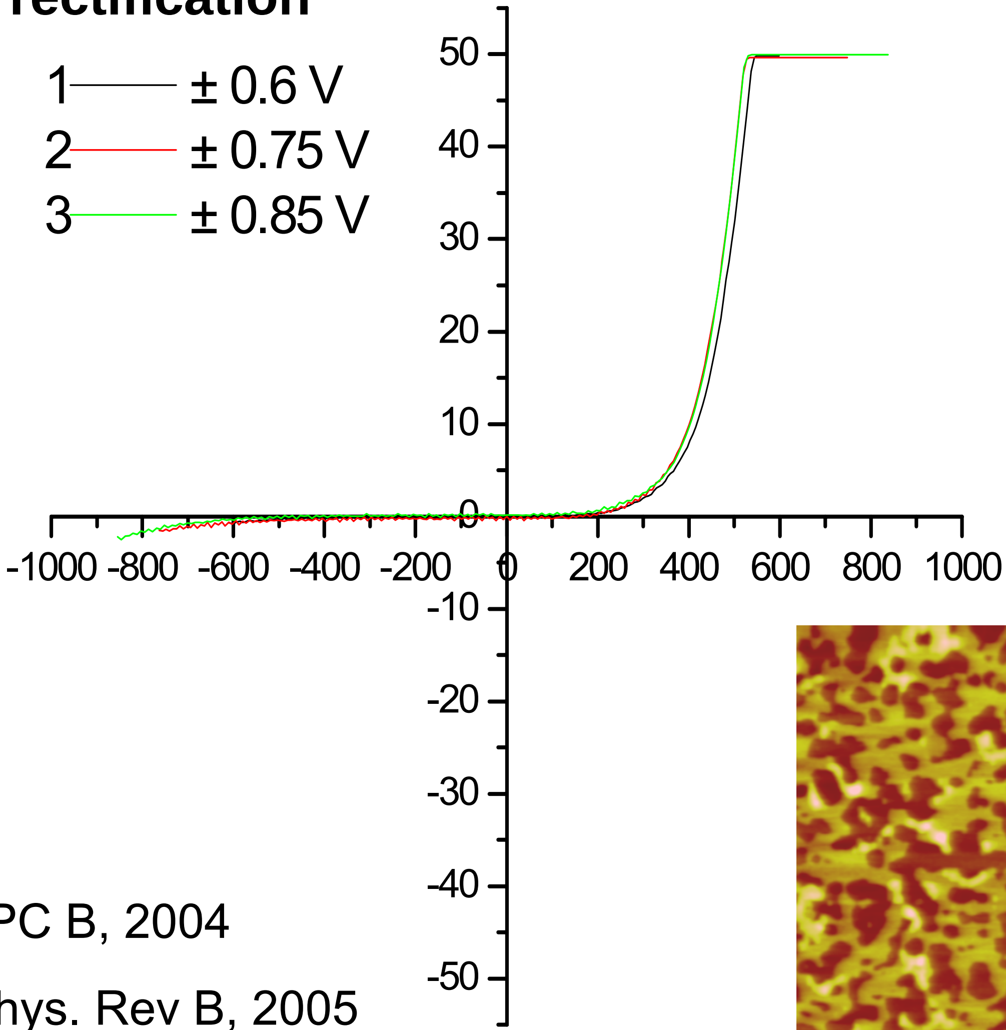


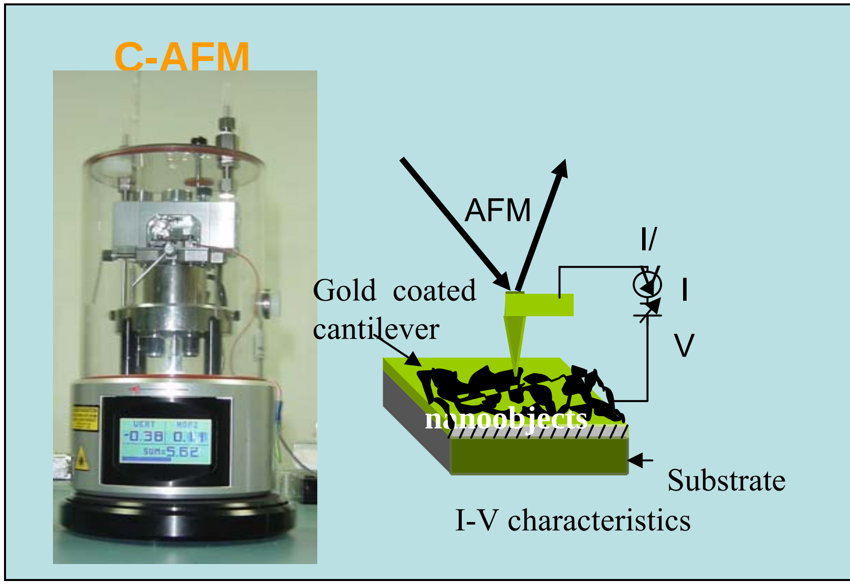


Pramana, 2005

• **Conducting - atomic force microscope** GUK-2

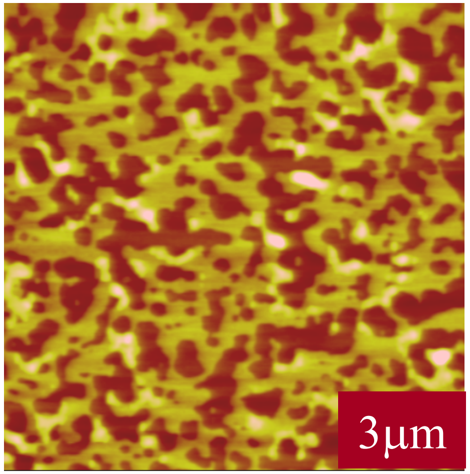
Metal-non metal bilayer showing rectification

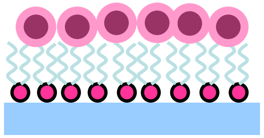




JPC B, 2004

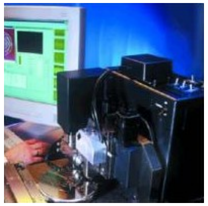
Phys. Rev B, 2005



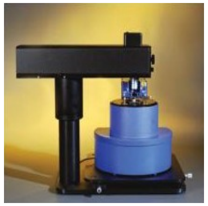


Si/GdSt/Au(3.5 mN/m)

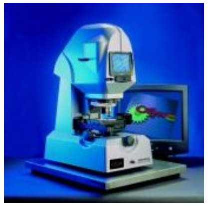
Veeco India Nanotechnology Laboratory, Jointly operated with JNCASR



Nano-man
High-end scanning probe microscope



The Digital Instrument CP-IITM scanning probe microscope



The NT1100, a bench top-Optical Profiler

Raman Spectroscopy, Brillouin Scattering and High Pressure Studies – Chandrabhas Narayana

Facilities

- Brillouin spectrometer
- Micro-Raman setup
- Diamond anvil Cell
- Low temperature setup

Materials studied and pursued

- Studies on manganites – CMR, Charge-ordering
- Low dimensional systems – fullerenes, nanotubes
- Pyrochlores, mid chain alkanes, Negative thermal expansion materials (like $ZrWO_4$)
- Proteins – p300 (HAT – cancer), cd4 (counts – HIV/AIDS)

Interests of the Laboratory

- Phase transitions in solids and liquids under pressure and temperature variations.
- Magnetic, acoustic and optical studies on solids
- Surface-enhanced Raman studies on Biological systems.
- High-energy x-ray studies of materials using synchrotron source.

Organic Electronic Devices: Physics & Mechanisms

- Field Effect Transistors
- OLEDs & Organic Solar Cells
- Optical Position and Image Sensors
- Organic Semiconductor-Nanoparticle/nanotubes Hybrid Structure

Photophysics of organic semiconductors

- Photoinduced charge separation in polymer blends and heterostructures.
- Spatially Resolved luminescence and current in hybrid structure using far-field and near-field photocurrent/ fluoroscence microscopy.
- Study of defect-states distribution and kinetics at interfaces and bulk.

Soft Matter Studies

- Electric Field induced patterns on elastomeric surfaces.
- Soft lithography procedures and conducting ink manipulation on surfaces

BioPhotonics and Electronics

Proton-transport in retinyl-membrane proteins/ conducting polymer structures: Biophysical features and device implications. *(ex. Artificial Retina).* Prepatterned polymer surfaces as templates or scaffolds for cell- trapping, growth and tissue engineering.

- Optical Control, amplification, Switching and Memory Effects in Organic FETs.
- Tunable Resonant Microcavity Structure for sub-gap amplification.
- 3% Organic Solar Cell
- Interesting biophysical and electrochemical activities at Conducting Polymer-Membrane Protein (bR) Interface.
- Sub-micron current contrast microscopy of polymer blends.
- Electric Field Patterning of Soft solid films
- Hybrid SWNTFET structures and Optically induced phenomena.

Materials Modeling and Theory

Shobhana Narasimhan: Surfaces, Catalysis, Clusters, Nanowires, *Ab initio* methods

Swapan Pati: Magnetism, Organic materials, Charge transport, Spintronics, Quantum Chemical and Many body calculations

Srikanth Sastry: Disordered systems, Dynamics, Liquids, Complex systems, Metastable systems, Statistical Mechanics

Balasubramanian Sundaram: Complex systems, Molecular materials, Green Solvents, Molecular Dynamics, *Ab initio* MD

Umesh Waghmare: Functional materials, Nanomaterials, Ferroelectrics, Mechanical properties, *Ab initio* methods

+ Additional JNC Faculty

Associate Members (around 20) to be drawn from across the country and abroad

Problems of Interest

- Nanoclusters: Structure, Stability, Nano/Bulk
- Nanodots on surface steps, nanocatalysis
- Properties of nanoscale objects (wires, tubes, ….)
- Charge transport in nanoscale systems
- Multiferroics
- Smart Structures: Mechanical properties
- Novel magnetic systems
- Non-linear optical materials
- Disordered materials: Landscape analyses
- Free energy methods to study phase transitions
- Mesoscale methods
- Biomaterials
- Complex systems

etc ..

Clusters: Structure, thermal properties, nanocatalysis, magnetic properties

Small, nanosized clusters are important/interesting:

Drive in nanotechnology to make smaller components

Novel properties that differ from that of macroscopic material

Determination of structure very difficult (large number of degrees of freedom); Plan to develop & explore new algorithms

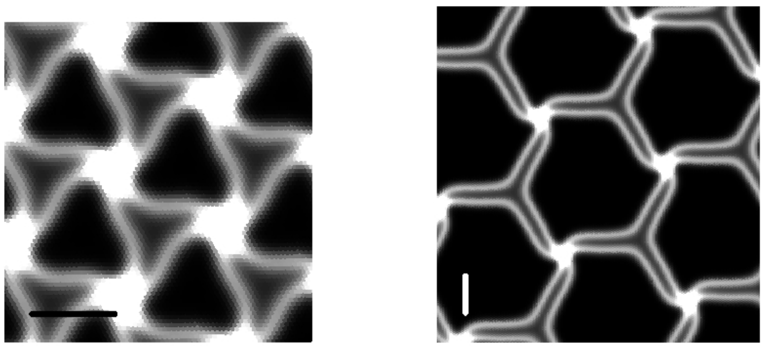
Thermal properties: how does melting temperature vary with size? (open question, small clusters less / more thermally stable than bulk material!); Plan to study using density functional perturbation theory and ab initio molecular dynamics

Magnetic properties: How do magnetic moment and magnetic anisotropy vary with cluster size and morphology? (applications for info storage)

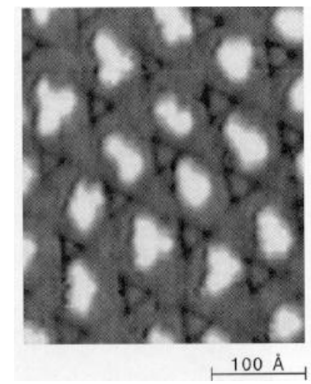
Nanocatalysis: Tune catalytic activity by adjusting size of cluster, design for maximum efficiency; will calculate reaction barriers using DFT

Surfaces: Patterning, Growth, Catalysis

- Reconstructed (~10 nm) metal surfaces as templates to grow self-organized arrays of magnetic nanodots; data storage?
- Use model potentials parametrized by *ab initio* calculations



Narasimhan & Pushpa



Brune et al.

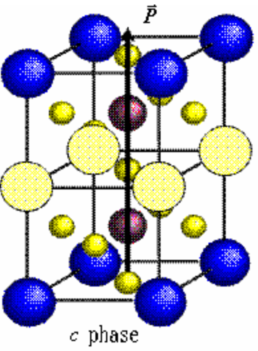
Simulated STM images of reconstructed Pt(111)   Fe islands on Ag/Ag/Pt(111)

- Heterogeneous catalysis: metal surfaces as catalysts, e.g., catalytic oxidation of CO, reduction of NO_x
- Mechanism and reaction barriers, focusing on mechanism of changes in surface geometry & the effect of local environment (defects, etc.) on catalytic activity

Phenomena at the Nano-scale

A. Ferroelectricity

A1

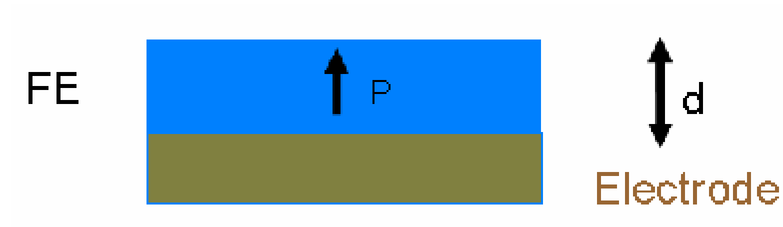


Nano-structured ferroelectrics:
Superlattices
Epitaxially tuned materials

Better piezoelectric properties

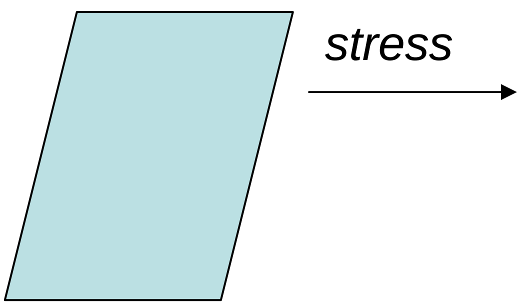
A2

Polarization Switching Dynamics in Ultra-thin (nano) FE Films



Switching: size (d) dependence

B. Mechanical Behavior



Mechanical failure is a singularly important factor in design of nano-scale devices:
How do the nano-objects break or plastically deform?

Determine how the presence of a surface affects unstable stacking fault energies and formation of dislocations

Studies of biferroic and lead-free ferroic materials

Materials that are simultaneously ferroelectric (FE) and ferromagnetic (FM): very rare

Transition metal oxides: d^0 ► FE d^n ► magnetism

Various mechanisms:

(a) ABO_3:- lone pair of electron of A cation: FE; transition metal B: FM. e.g. $BiFeO_3$

(b) Improper FE (originated by symmetry), transition metal: FM. e.g. $YMnO_3$

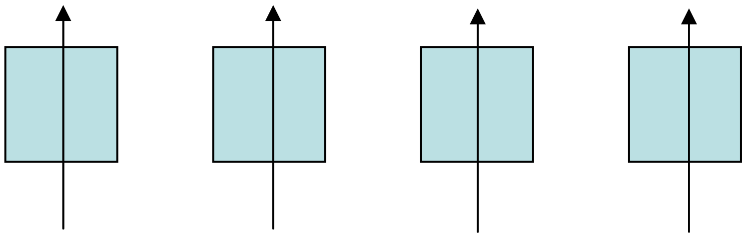
(c) Magnetoelastic coupling (primary order parameter) giving rise to FE. e.g. $TbMnO_3$

(d) Superposition of distinct charge ordering break centrosymmetry! e.g. $(LaCa)MnO_3$

Focus on materials belonging to categories (a) and (b) and others.
In close collaboration with experimental group of Prof CNR Rao.

Nonlinear Optics

Parallel orientation of the dipolar molecules.

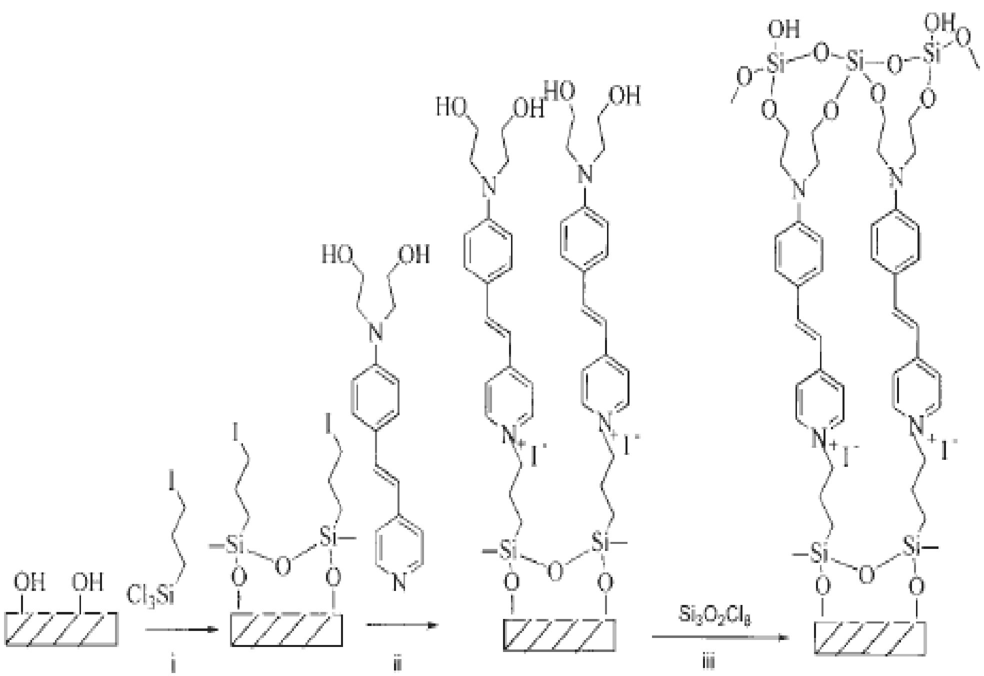


Produces the maximum NLO response

Self Assembly techniques

Molecular modular assembly technique:

Produces excellent control over film thickness and structure with long-term stability

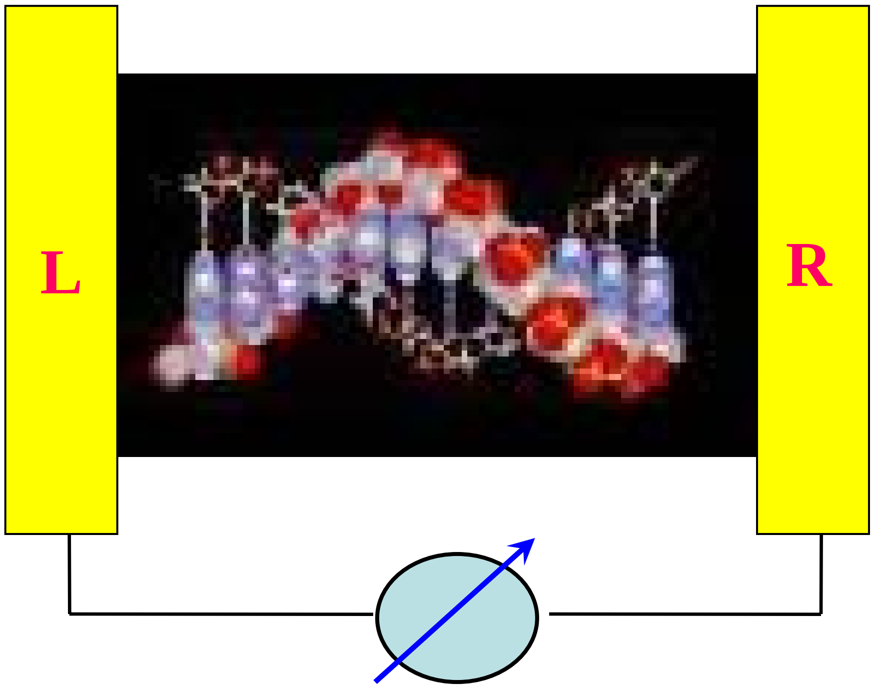


Dipolar interactions :

Hydrogen bonds :

What are the essential parameters at this length scale to design materials for effective device applications?

Biomaterials



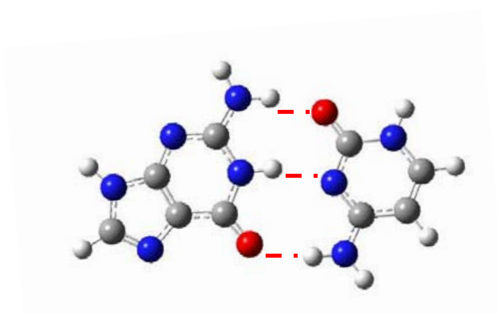
Can DNA be used as a transistor ?

↓

Conductance through DNA depends crucially on the sequence of the base pairs.

↓

Microscopic details of π-stacking and H-bonding interactions between the base pairs are crucial for a proper understanding of transport mechanisms.



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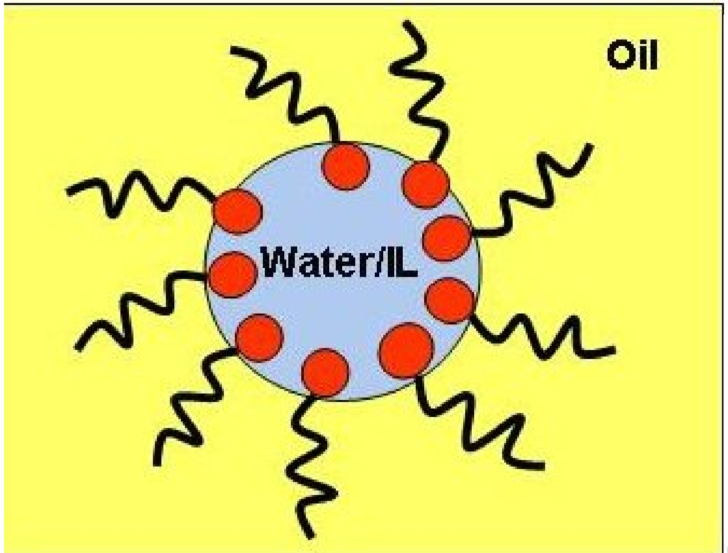
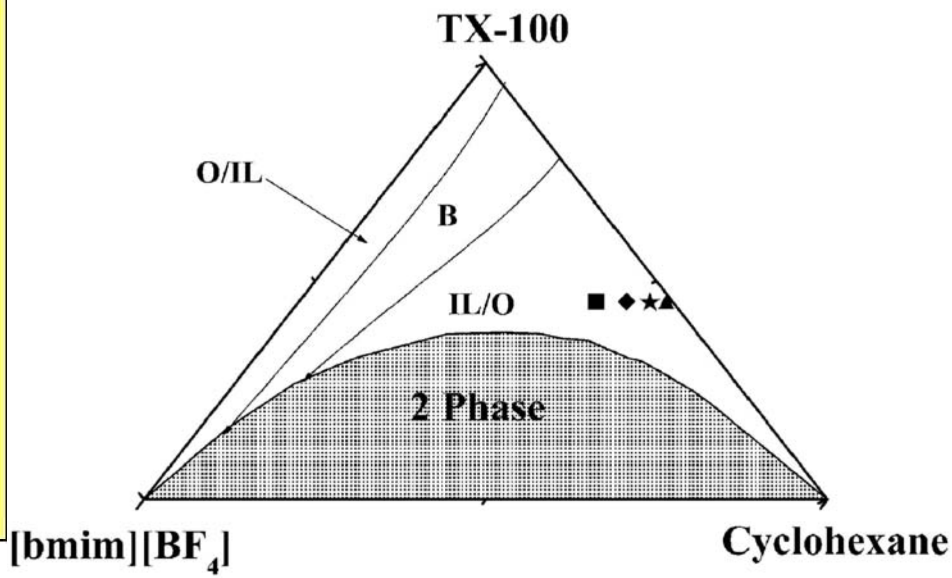
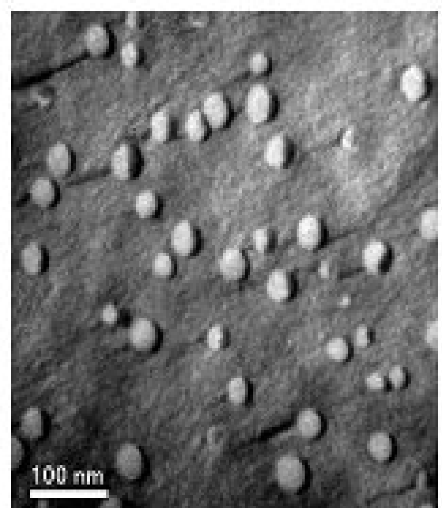
We are interested in providing answers to such questions from first principle calculations, which will essentially help in understanding the radiation damages and mutations of DNA .

Complex Systems: Microemulsions





Plan: MD studies of polar cores used for nanoparticle synthesis

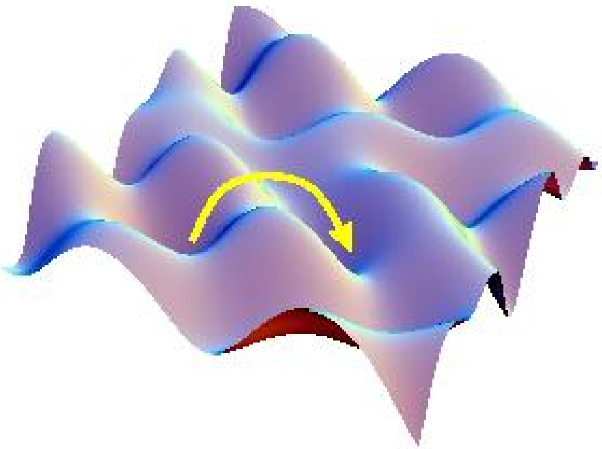


Freeze dried TEM

Buxing Han's Group

Disordered and complex systems

- Accelerated simulation methods for glassy systems: liquids, colloids, polymers, biomolecular systems
- Methods for energy landscapes: Saddle point search, reaction path, global optimization, phase transformation
- Free energy estimation of condensed systems
- Mesoscale modelling: Multi-scale modelling methods, protein aggregation



Building Realism: Ways and Means

Many Body Methods: DMFT, DMRG, QMC, Strongly correlated systems

Density Functional Theory: One electron theory, Grid based, Plane waves/Localised Basis

Quantum Chemistry: Semi-Empirical, Molecular interactions

Molecular Dynamics/Monte Carlo: Empirical potentials, Atomistic/Coarse Grained

Analyses: Energy Landscapes, Dynamical Matrix, Voronoi tesselations, Bonding characterization using Geometric phases, …

Ab initio MD: DFT + MD, Potential on-the-fly

Quantum Dynamics: Many body + MD

Large scale computation on realistic representations of materials

Energy: 1kcal/mol – Few eV
Length: 0.1 nm – μm
Time: fs - ms

INTENSIVE CPU, LARGE MEMORY & STORAGE REQUIREMENTS
PARALLEL IMPLEMENTATIONS
ESSENTIAL

Facilities/Programmes of CCMS

Infrastructure

A high performance computing platform (256 CPUs or more, with a low latency network) + necessary support infrastructure and software tools

Schools, Workshops, Short-term courses (2 *p.a.*)

A teaching cum hands-on sessions laboratory with around 30 PCs that can be clustered

Visitorships

Support University researchers and others to visit CCMS, use the facilities and to interact with peers

Conferences

One international conference on CMS per year

- Thank You - Namaste