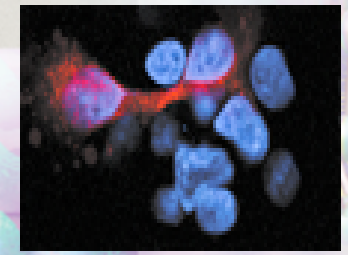
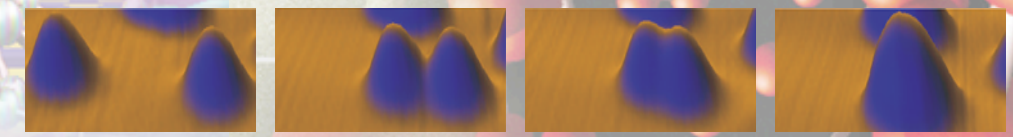
Molecular FOUNDRY
A NANOSTRUCTURES USER LABORATORY

THE MOLECULAR FOUNDRY

A Nanostructures User Laboratory At Berkeley Lab

JEFFREY BOKOR
Deputy Director
jbokor@lbl.gov





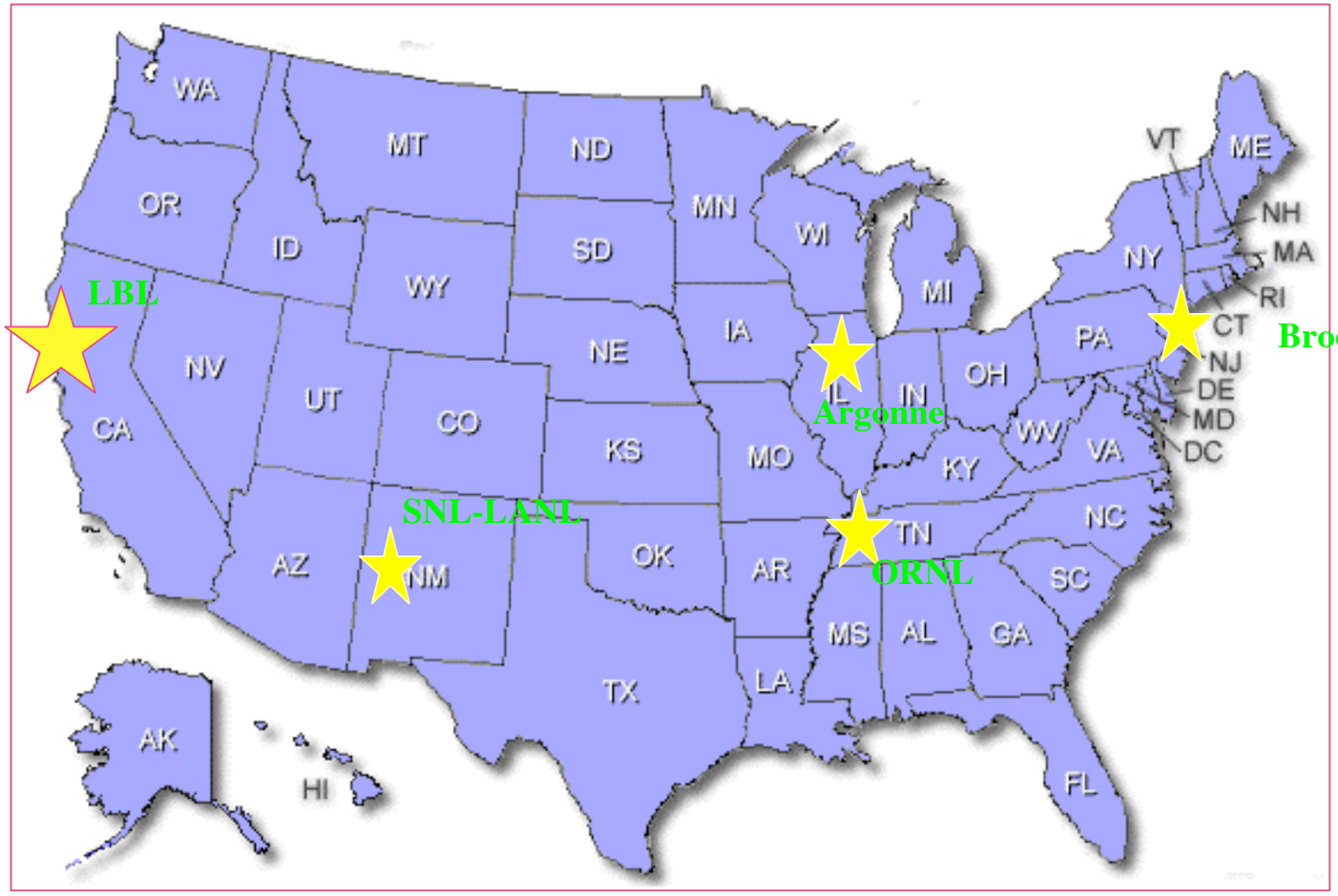
Office of Science
U.S. DEPARTMENT OF ENERGY

What will you learn today?

- The Molecular Foundry – an NSRC. What is that?
- What sort of research can be done at the Molecular Foundry?
- What is the status of the Project?
- What are the opportunities for collaborative use of the Molecular Foundry and the ALS?

DOE Nanoscale Science Research Centers

5 Centers located near light sources or neutron scattering facilities.

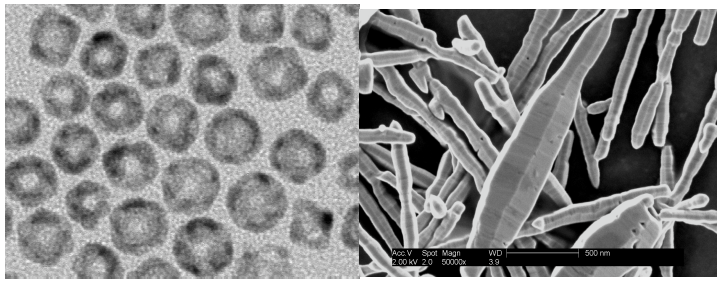


Mission

- National User facility for nanoscale science
- Enable Users to design, synthesize, and characterize state-of-the-art materials
- Provide Users rapid access to cutting-edge techniques and training
- Create dynamic environment for collaborative research
- Provide means to solve important problems in energy science

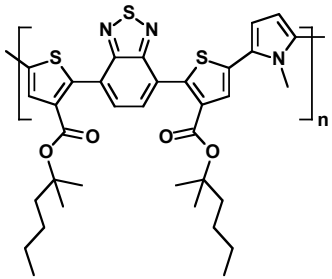
Molecular Foundry Facilities

Inorganic



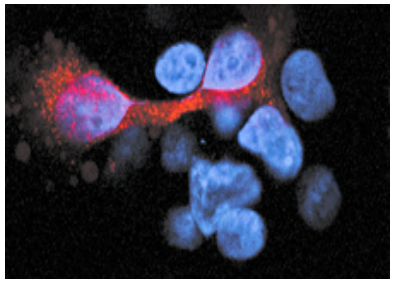
A. Paul Alivisatos

Organic



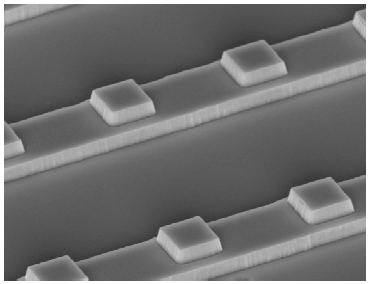
Jean Fréchet

Biological



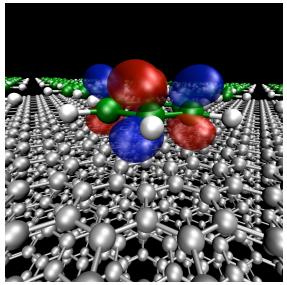
Carolyn Bertozzi

Nanofabrication



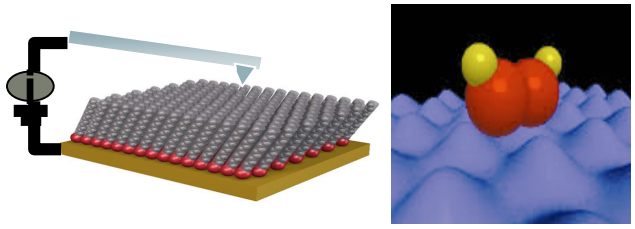
Jeffrey Bokor

Theory



Steven G. Louie

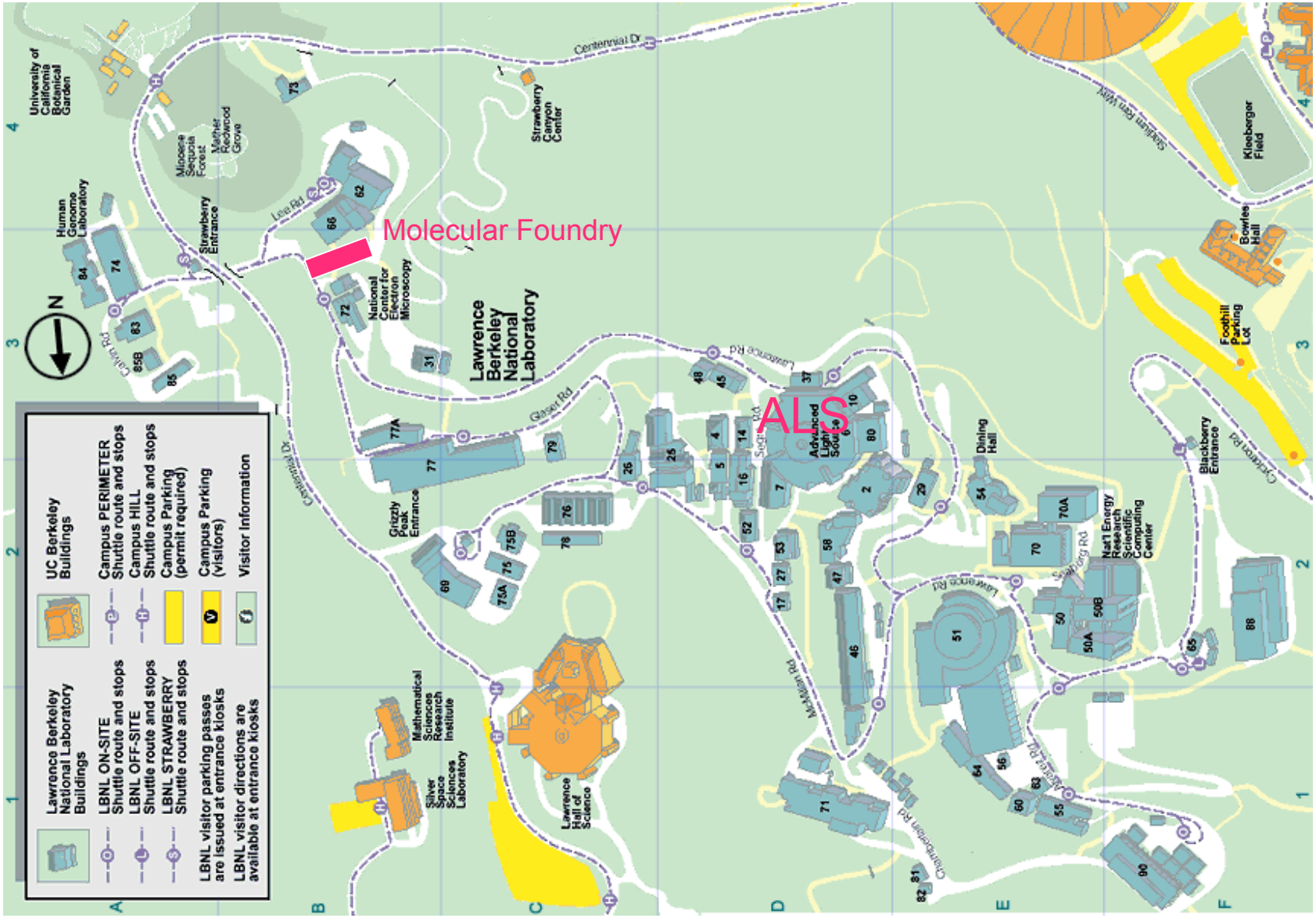
Imaging & Manipulation



Miquel Salmeron


2005 10 5

Foundry Location

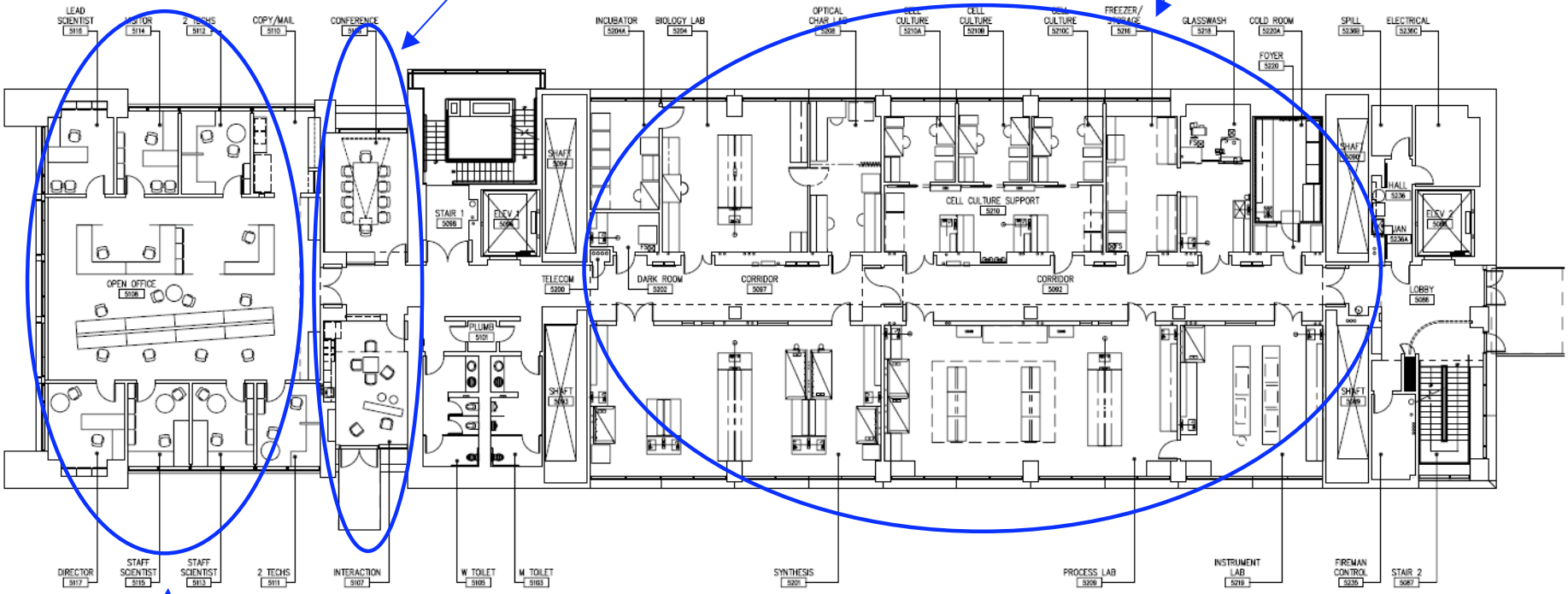


The Molecular Foundry — a user facility for nanoscale materials

TMF – 5th Floor Upper Levels

Conference / Interaction space

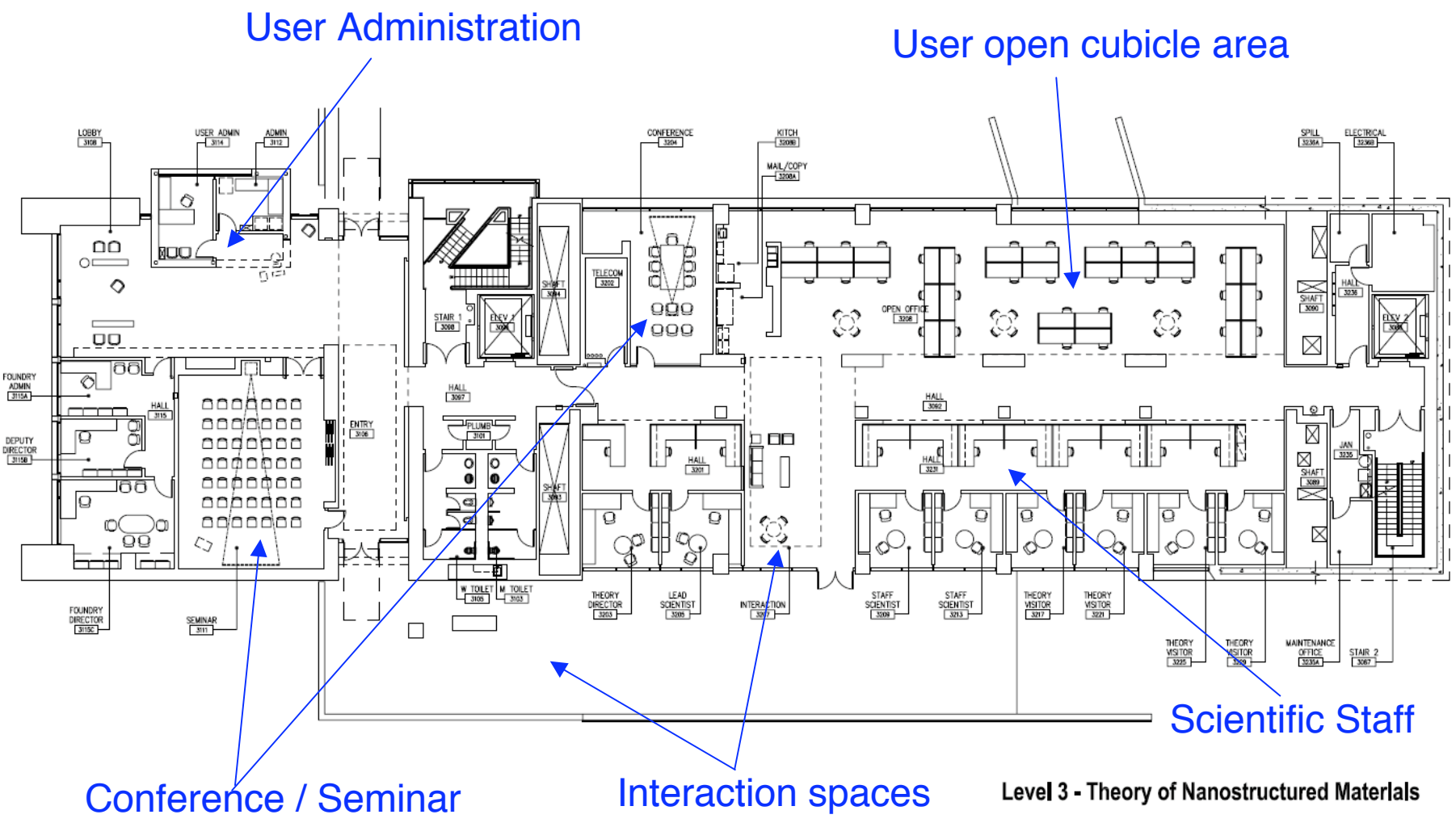
Laboratory space



Office space

Level 5 - Biological Nanostructures

TMF – 3rd Floor
Primary User Access Point



Facility description

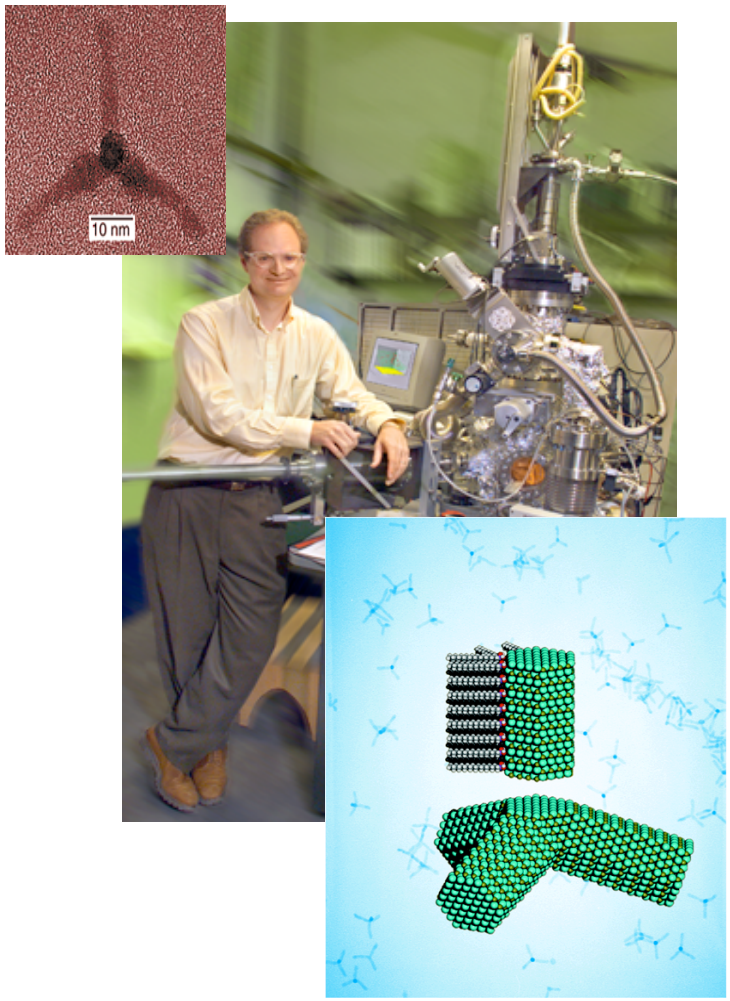
- State-of-the-art instrumentation
- Technical support staff
- Collaborative scientists to support users
- Internal research program
- Projects selected through peer review
- No charge for non-proprietary research

Types of Foundry projects

- Obtain nanostructures
- Create new nanoscale materials/devices
- Learn to use new methods
- Develop new methods
- Learn to replicate new instruments/ techniques
- Pursue long term collaborations

Inorganic nanostructures

Prof. A. P. Alivisatos, Facility director

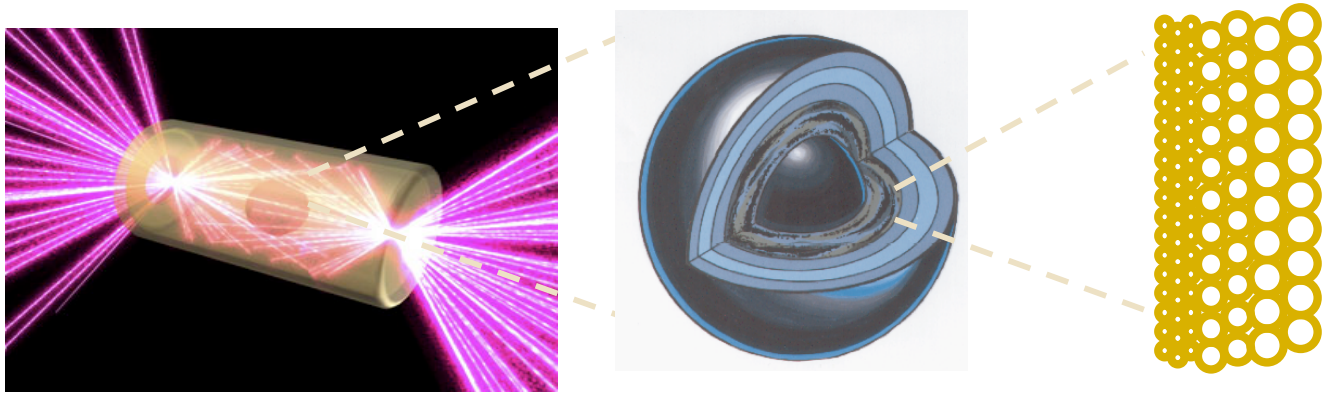


Current capabilites

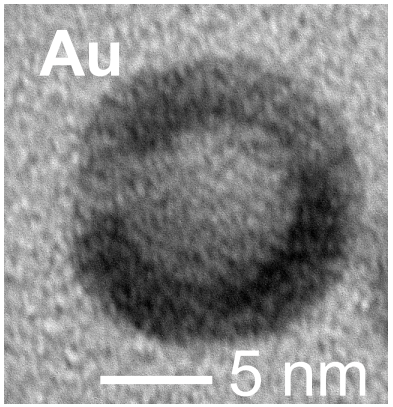
- Nanotube synthesis
- Nanowire synthesis
- Colloidal nanocrystal growth

Associate directors:
Peidong Yang, Alex Zettl

Targets for LLNL's National Ignition Facility (NIF)– Incorporating Hollow Nanocrystals



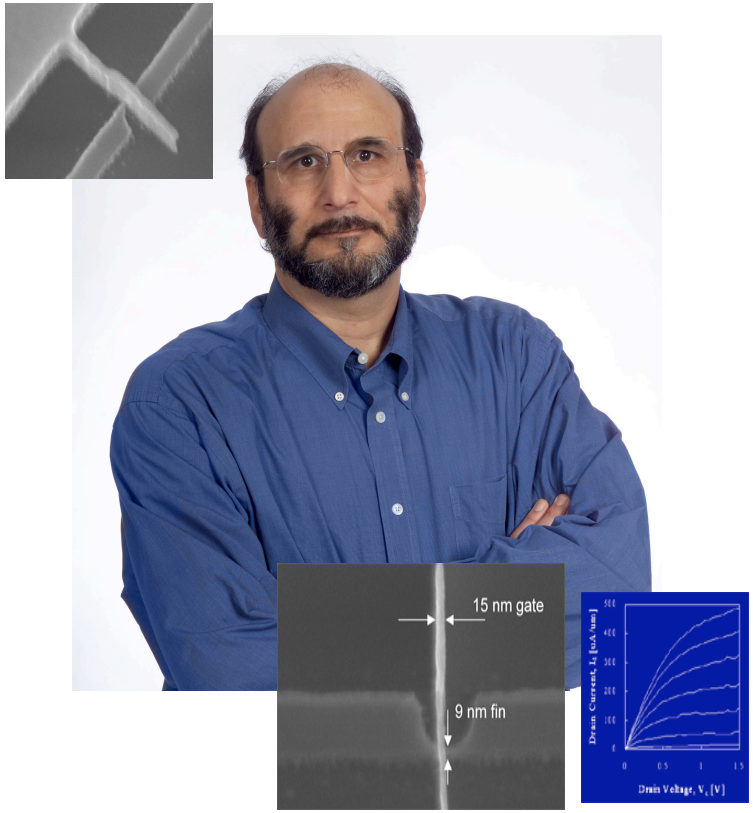
- NIF's 192 laser beams are designed to produce 1.8 megajoules of energy and 500 terawatts of power.
- High Z metals with low density are needed to independently control opacity and hydrodynamic propagation.
- Foam with variable density allows energy to be coupled into the inner shell over a fixed depth thereby controlling Raleigh-Taylor instabilities.



To prevent instabilities during shock propagation, hollow gold nanocrystals have the advantages: 1) high Z, low density; 2) graded density is possible; 3) foams can be cast into arbitrary shape

Nanofabrication

Jeffrey Bokor, Facility director

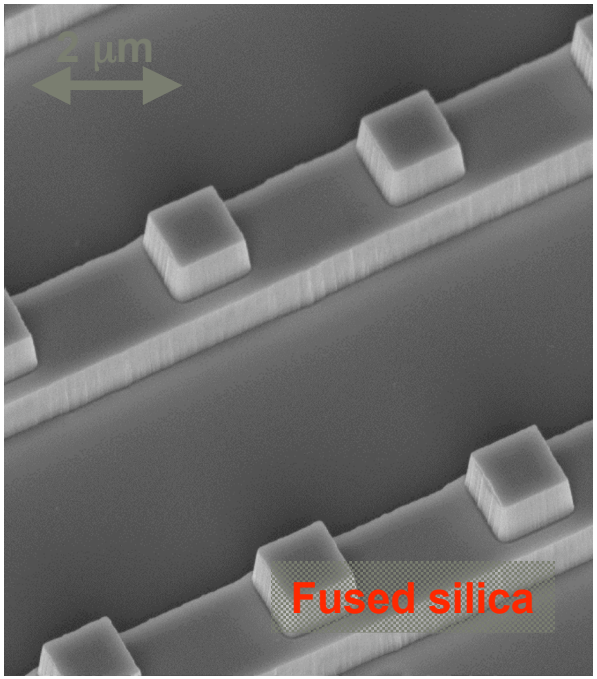


Current capabilities

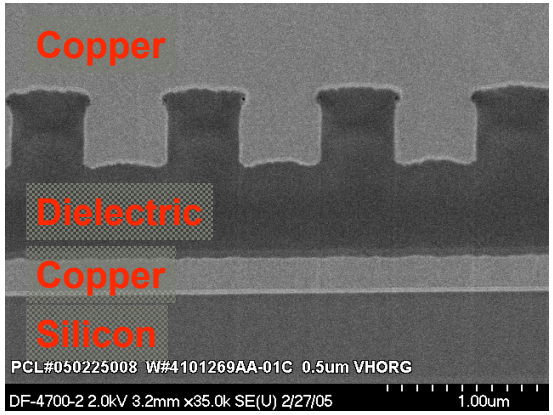
- High-resolution nanolithography
  - e-beam lithography
  - Nano-imprint lithography
  - Photolithography
- Process & techniques relevant to the integration of semiconducting materials with chemical & biological nanostructures

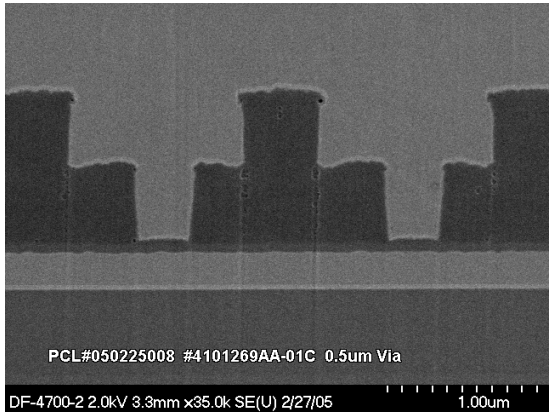
Nanofabrication: Imprint Lithography

Imprint template made at the Molecular Foundry



Interconnect structures formed with imprint lithography



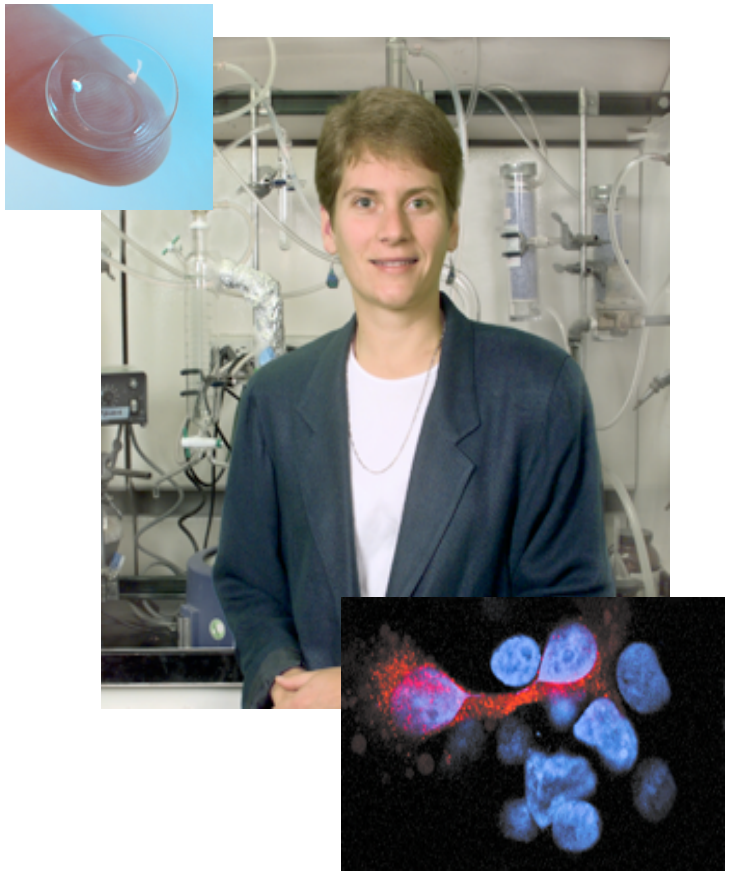


User: Grant Willson, UT-Austin

In collaboration with Molecular Imprints Inc., SEMATECH, and Motorola

Biological nanostructures

Prof. Carolyn Bertozzi, Facility director



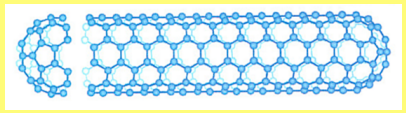
Integration, assembly, and testing of biological nanomaterials

Current capabilities

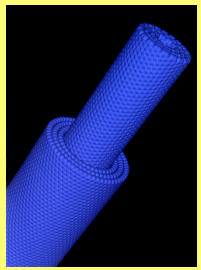
- Mammalian cell culture
- Bioconjugation chemistry
- Cell immortalization via telomerase expression
- RNA preparation and microarray analysis
- Phage library display
- Preparation of functional organic-inorganic nanocomposites

Probing the interaction between nanoscale materials and cells

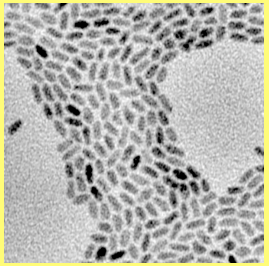
Size/shape-dependent effects



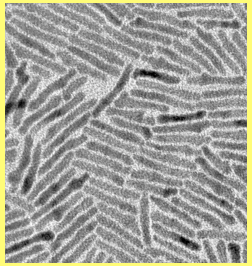
SWCNT



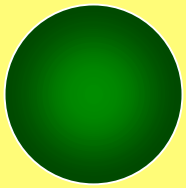
MWCNT



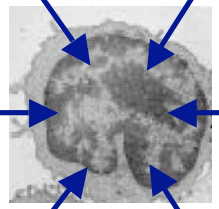
100 nm



Quantum rods with varied shapes and sizes

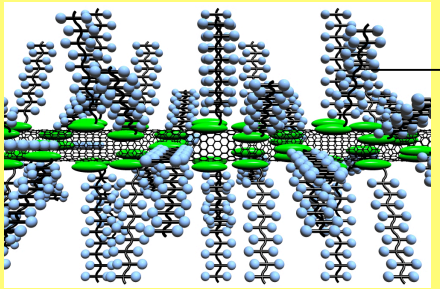


Quantum dots with varied sizes and colors

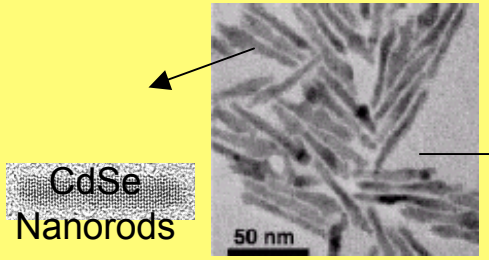


Healthy human cells

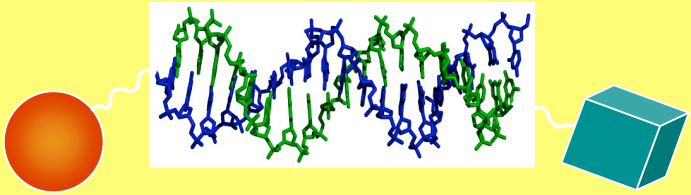
Chemical modification-dependent effects



CNT with biomimetic coatings



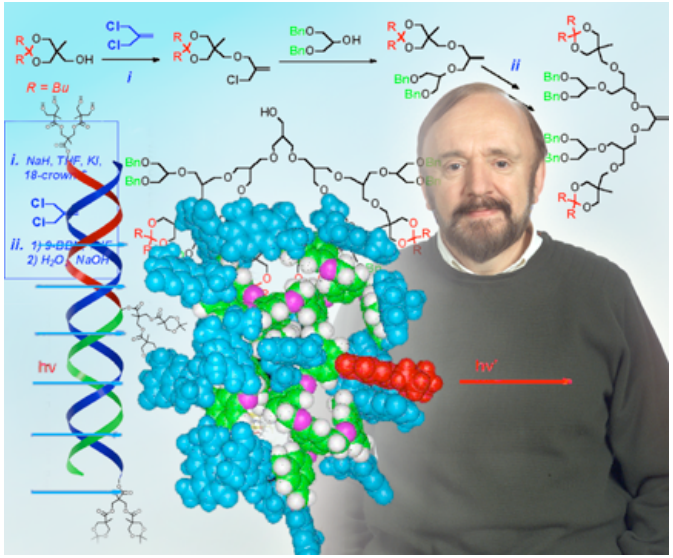
CdSe nanorods in poly(3-hexylthiophene)



Quantum dots conjugated with biomolecules

Organic nanostructures

Professor Jean Fréchet, Director

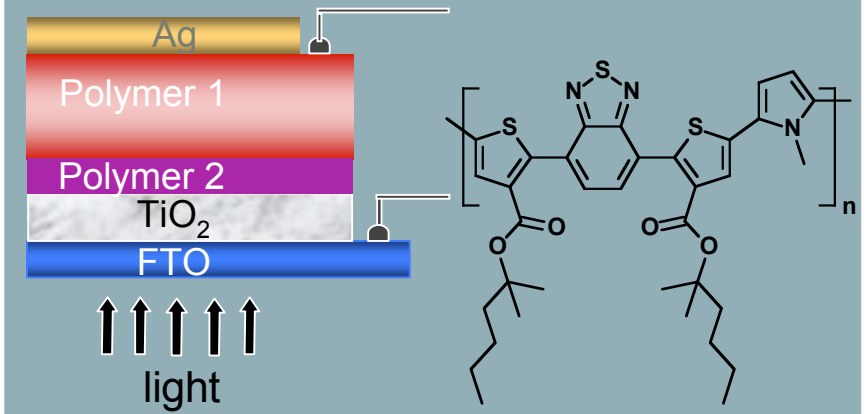


Design, Synthesis and Characterization of Organic Molecules & Polymers:

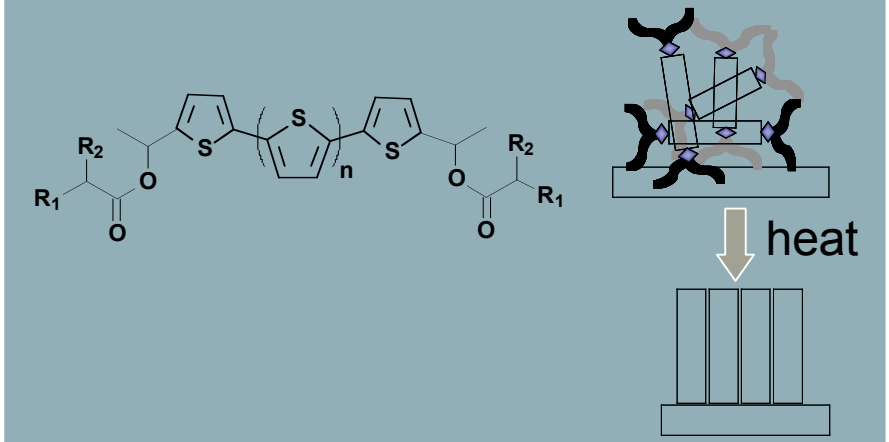
- Electroactive organic molecules
- Semiconducting oligomers and polymers
- Light Harvesting Materials
- Reactive surfaces, surface modification
- Organic Nanomaterials (organic nanoparticles, functional macromolecular assemblies, polymers)

Examples of organic nanostructures

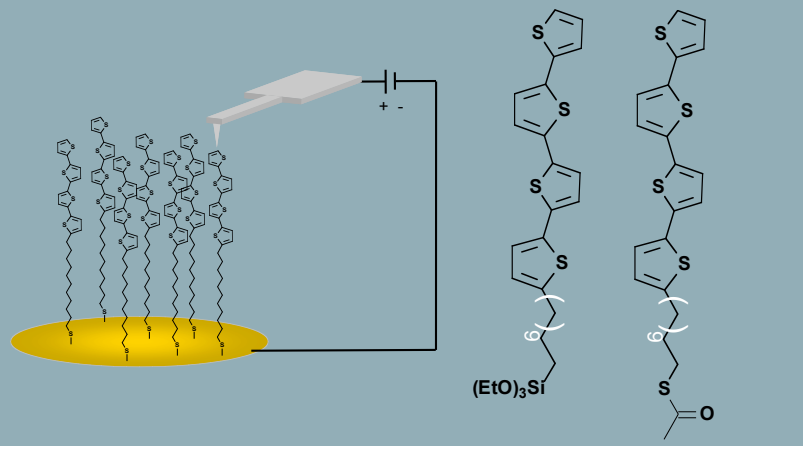
Polymers for Organic Photovoltaics



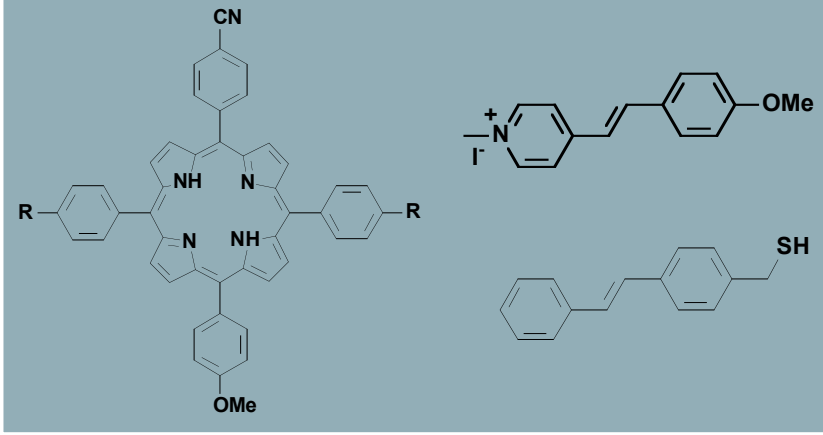
Oligomers for Organic-based Transistors



Oligomers for Surface Functionalization



Small Conjugated Molecules



Imaging and Manipulation

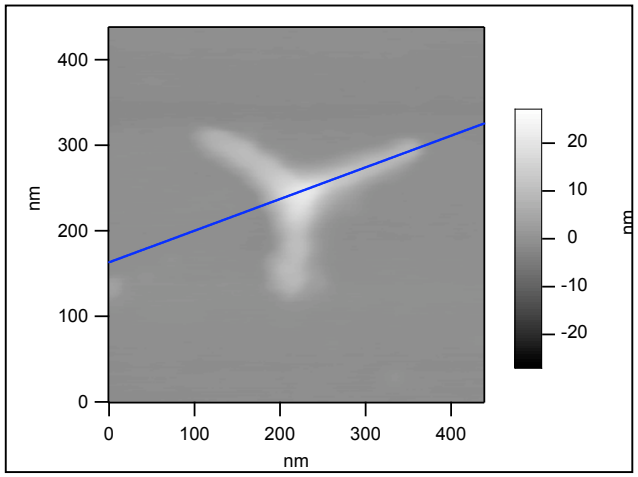
Miquel B. Salmeron, Facility director

- **Present capabilities**
  - UHV contact AFM for friction and conductance measurements
  - Ambient AFM with 2 nm resolution in tapping mode for soft matter

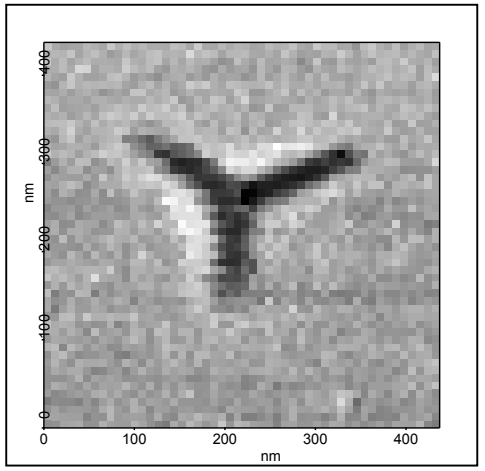
- **Future capabilities**
  - UHV 4 K STM
  - FIB nanofabrication
  - Scanning Raman
  - Ultra sensitive AFM for force profiling

Mechanical Properties of CdSe Tetrapods

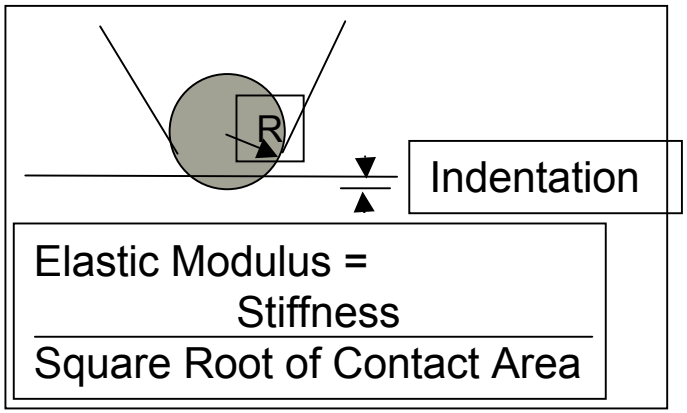
Topography



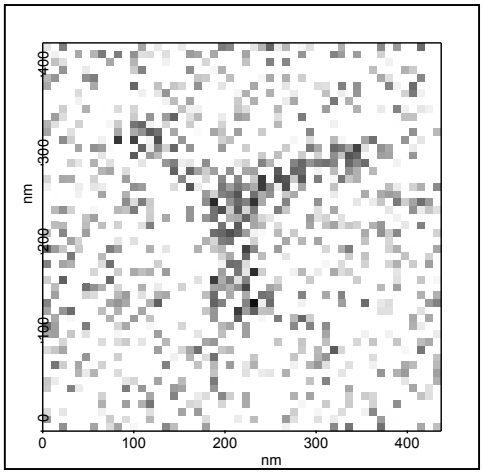
Adhesion Force Mapping



Hertz's Model

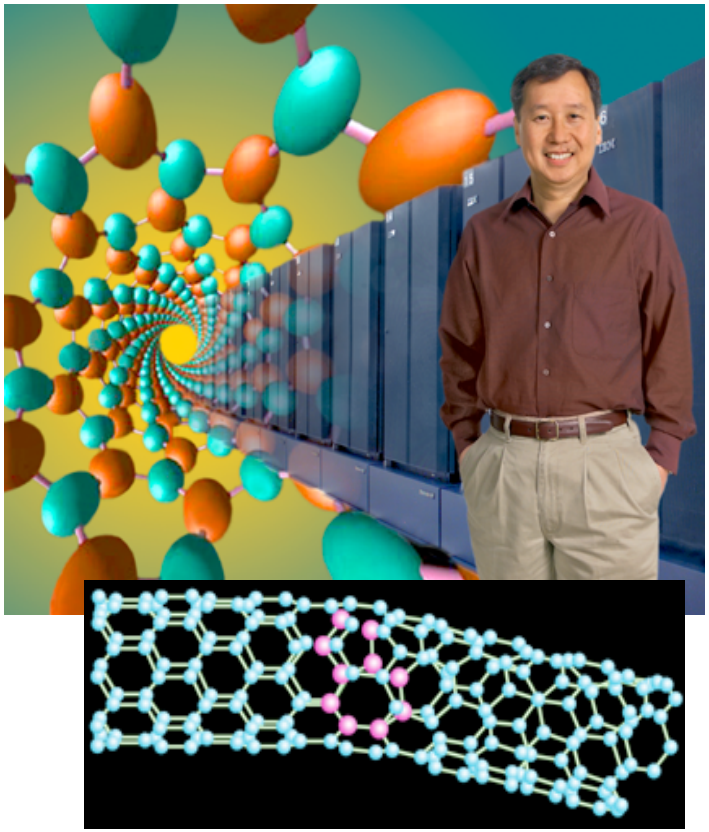


Young's Modulus ~ 80 Mpa



Theory of nanostructures

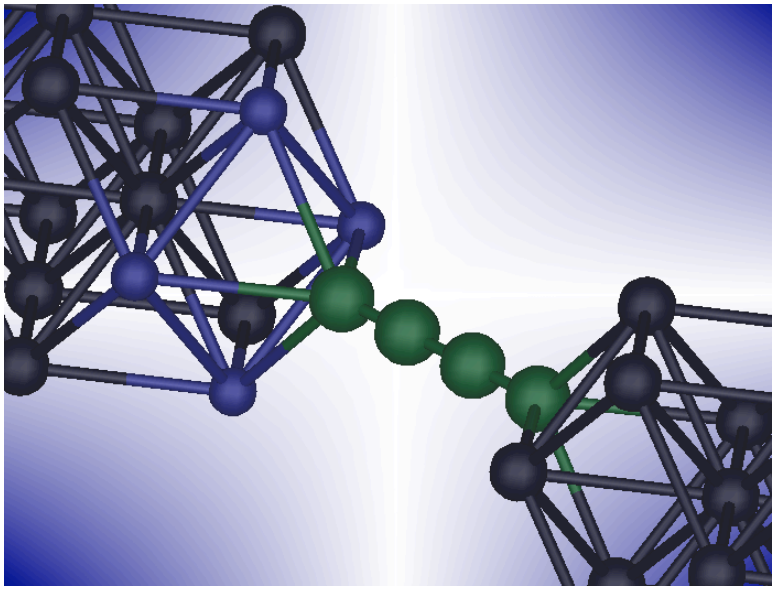
Steven G. Louie, Facility director



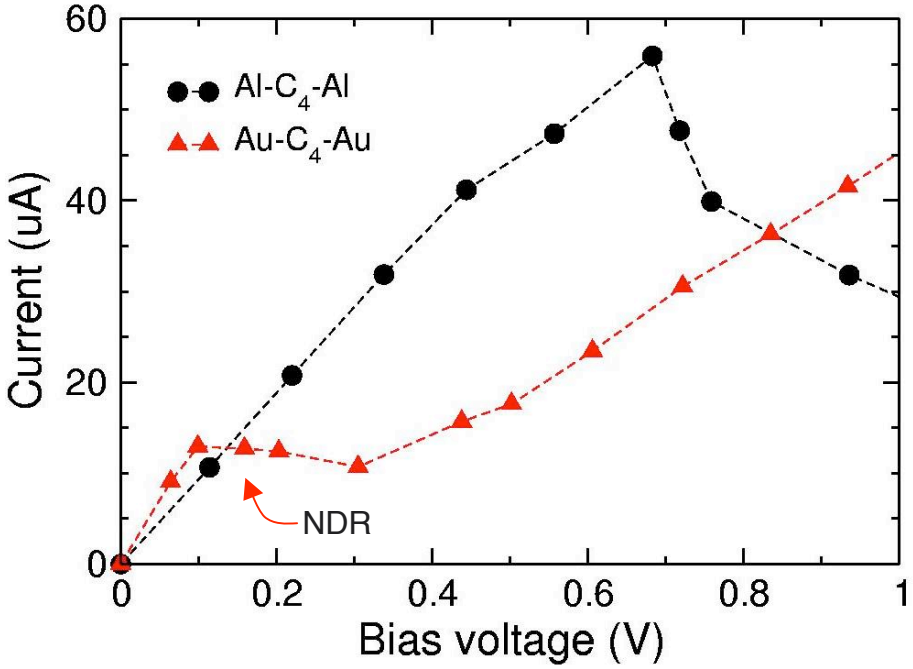
- First-principles density-functional theory
- Classical & *ab initio* molecular dynamics
- Excited-state properties with the GW/Bethe-Salpeter equation approach
- Electron transport at finite bias with a first-principles scattering-state method

Carbon chain: interesting benchmark

Carbon atomic wire between Al or Au leads



I-V characteristic



Chain resistance and I-V characteristic depend on the leads

Neaton, Khoo, Spataru, Louie, Comp. Phys. Rep., in press (2005)

Schedule

• Foundry "Jump Start"	Current operation
• Building Occupancy	January, 2006
• Initial Operation	March 2006
• Full Operation	October 2006

Molecular Foundry current activities

- **"Jump-start" program in place:**
  - **12 postdocs/scientists hired for 6 facilities**
  - **Actively hiring now for permanent scientific staff.**
  - **On schedule for opening in March of 2006**

For more information:

foundry.lbl.gov

Call for proposals!

Molecular FOUNDRY
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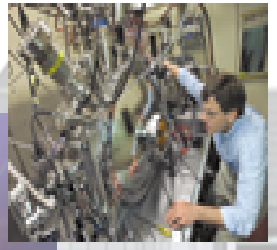
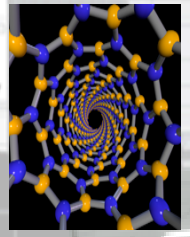
THE MOLECULAR FOUNDRY

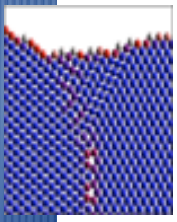
Facilitated Access to other LBNL User Facilities



ADVANCED LIGHT SOURCE

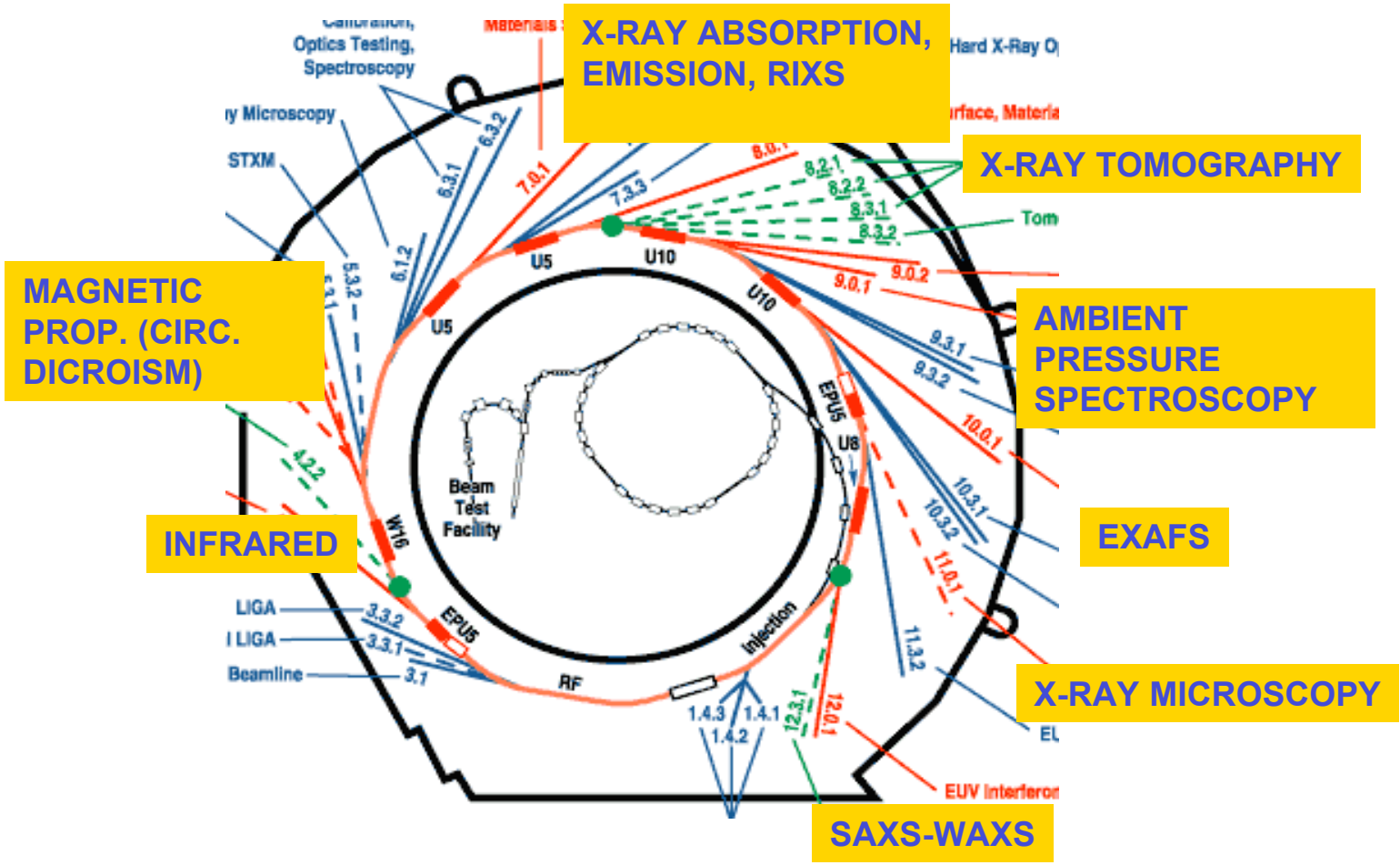


NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER



NATIONAL CENTER FOR ELECTRON MICROSCOPY

ALS Techniques of Interest for nanoscience



First TMF-ALS Joint Workshop

Soft X-Ray Scattering from Hard and Soft Matter

September 30, 2005

Building 66 Auditorium, Berkeley Lab

Sponsored by the Advanced Light Source and the Molecular Foundry, Berkeley Lab

Organizers: J. Kortright (ALS), H. Ade (NC State), J. Bokor (TMF)

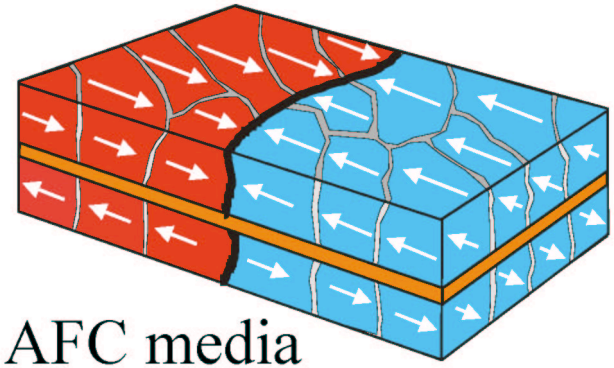
Workshop goals: Define impact, uniqueness

- Develop compelling scientific case for a world-class beamline facility for resonant scattering studies of nanometer-scale structure in a broad range of materials:
  - magnetic, correlated electron, multifunctional systems,…
  - polymers, liquid crystals, bio-materials,…
- Establish general technical specifications for beamline.
- Discuss optimal end-stations for these studies.

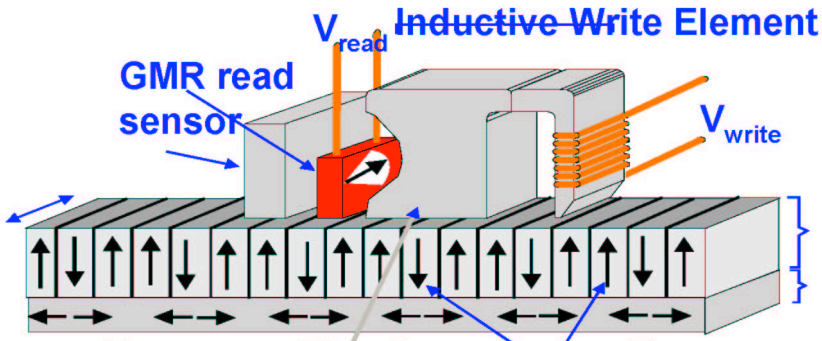
Why q-resolved scattering with soft x-rays?

- Dipole transitions to Fermi edge or anti-bonding molecular orbital states.
  ⇒ Unique, new scattering contrast mechanisms.
- Strong resonant lines
  ⇒ Scattering from *very* small volume of material
- Spatial resolution ~ λ/2: 1 nm up to several mm.
  Angles 10 x larger for given q ($q = 4\pi\sin\theta/\lambda$)
- Heterogeneity in what chemical/functional properties?
  - electronic structure (bands, bonds, anisotropies, …)
  - optical absorption/emission (PVs, LEDs, etc.)
  - magnetism
  - ferroelectricity (polarization)
  - piezzoelectricity (strain)
  - self-assembly, dynamics

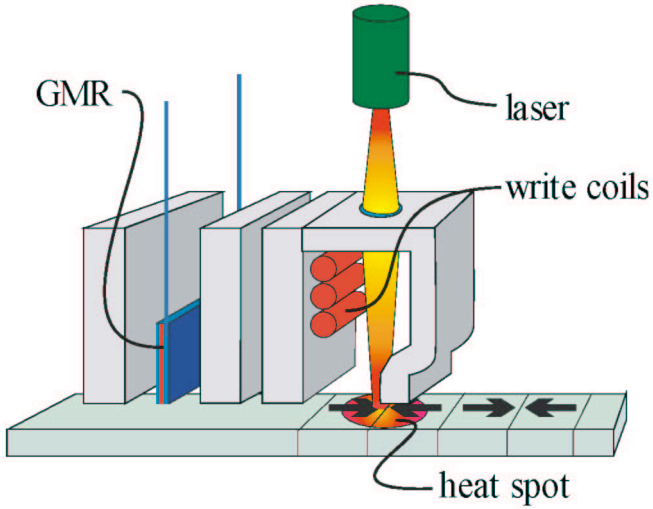
Advanced media and systems



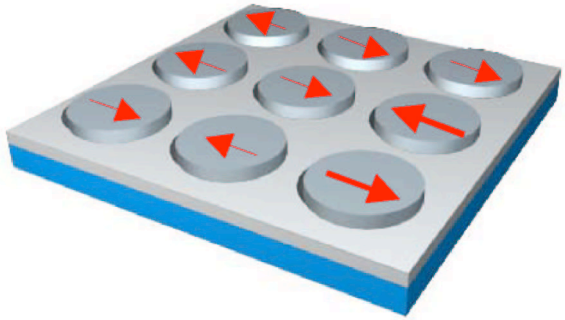
AFC media



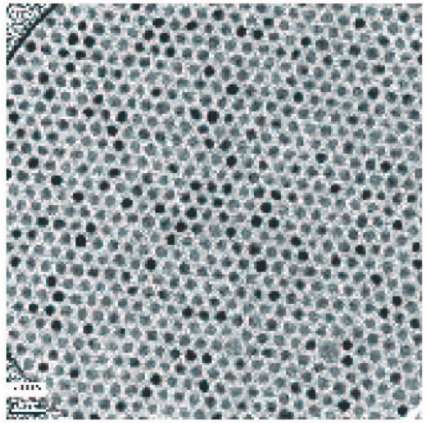
Perpendicular recording



Thermal assisted recording



patterned media



S. Sun, IBM

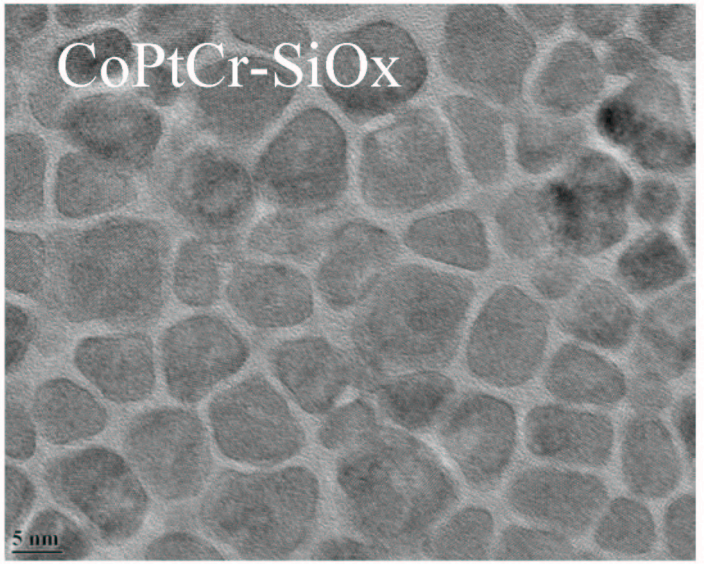
self-organized media

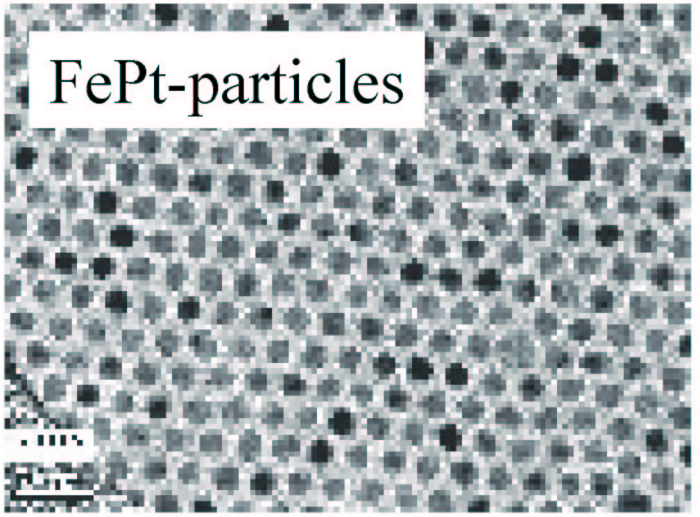
Moser et al., J. Phys. D: Appl. Phys. **35**, R157 (2002).
Terris and Thomson, J. Phys. D: Appl. Phys. **38**, 199 (2005).

E. Fullerton, Hitachi

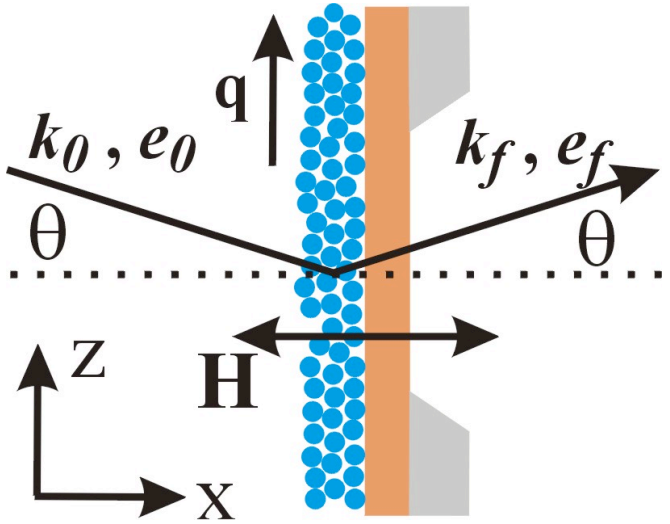
Nano 'issues'

- control of nano-structural order
  - chemical segregation
  - layered heterostructures
  - lithography
  - self-assembly
- link structure/magnetic
  - Short-range exchange
  - Long-range dipolar
- thermal energy
  - spin wave modes of small structures
  - collective modes
- high current densities
  - dipole fields, spin torques, heating
- sub-ns reversal
- particle-to-particle variations
- particle-to-particle interactions



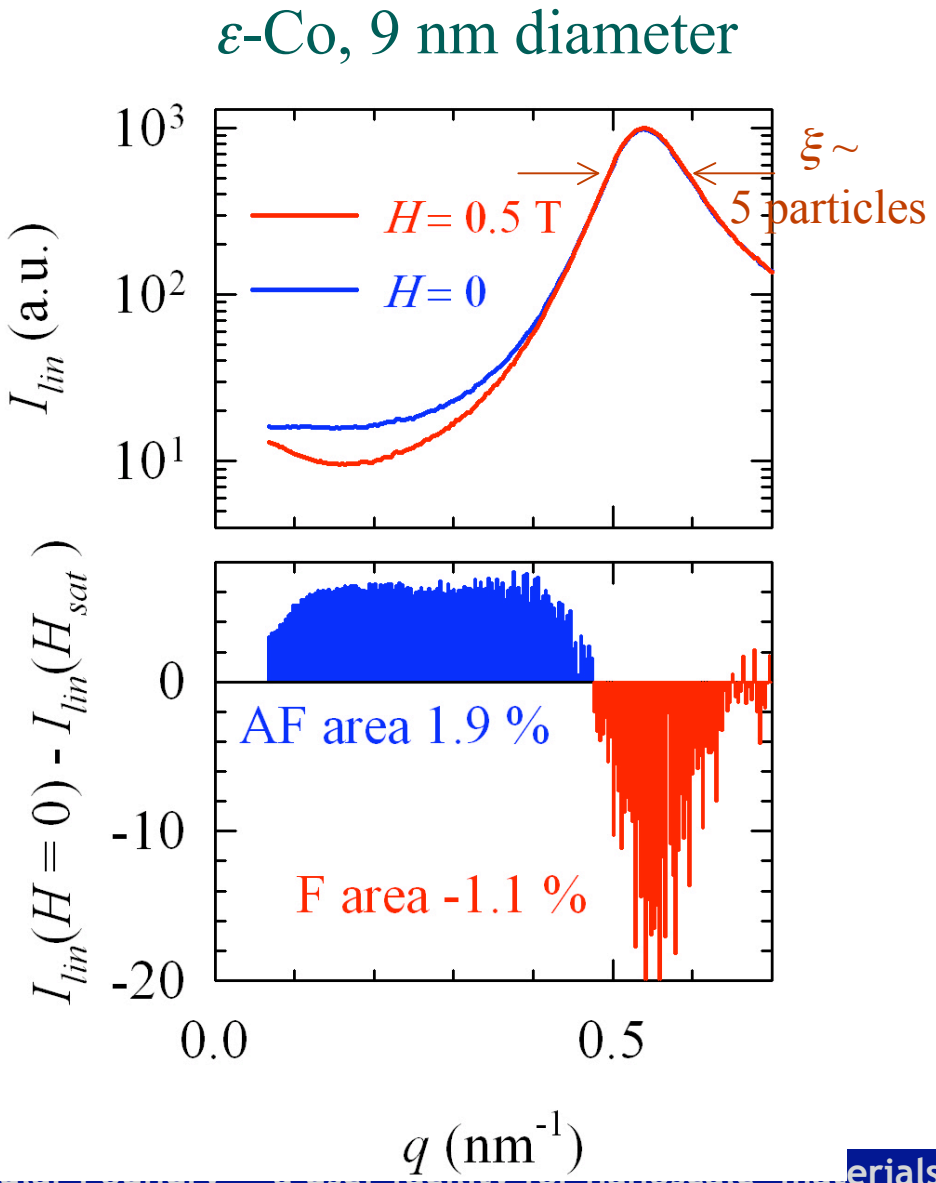


Example: Dipolar interactions in dense Co nanoparticle assemblies – are they significant?



$$I_{lin}(q,H) = I_{charge-charge}(q) + I_{mag-mag}(q,H)$$

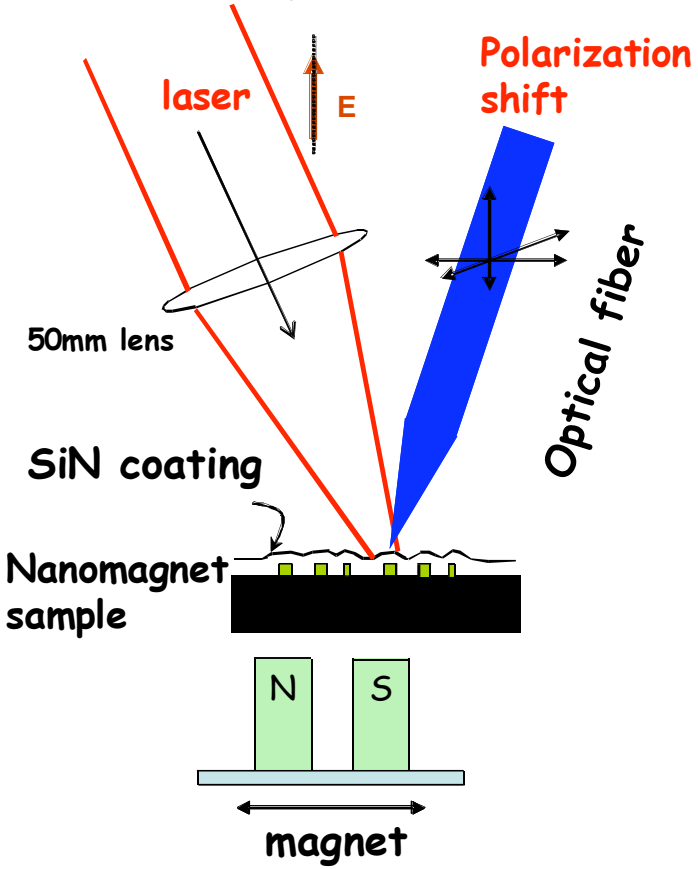
$\Delta I_{lin}(q,H)$ gives remanent paramagnetic scattering.



J. Kortright, LBL

Dynamic Characterization of Nanomagnets

Naser Qureshi, Holger Schmidt UCSC

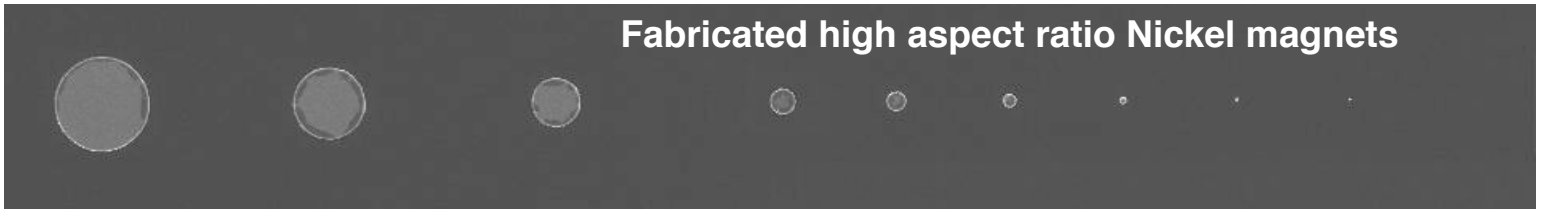


Objectives:

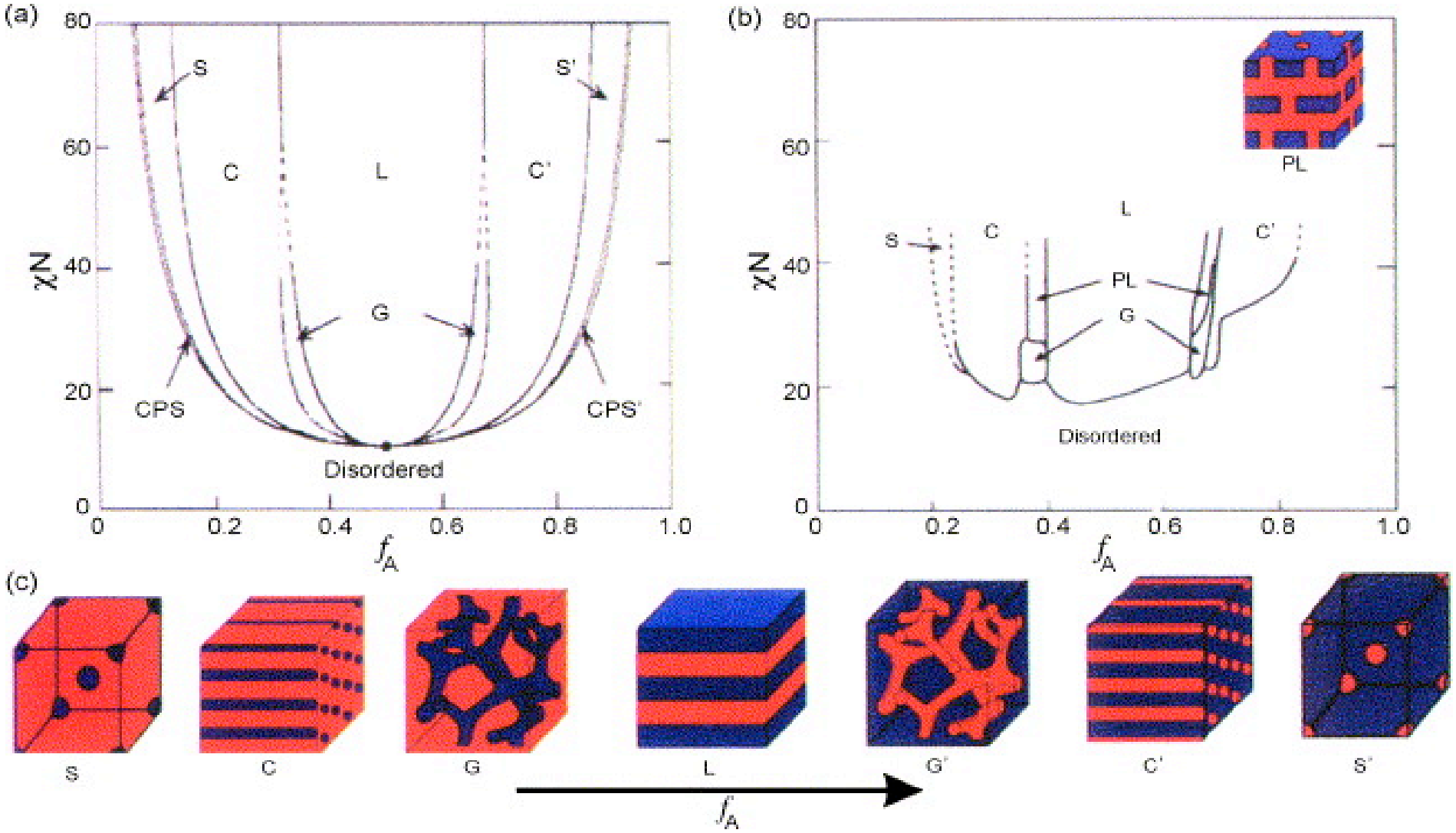
- **Time-resolved near field optical characterization of magnetization reversal on single-domain nanomagnets using magneto-optic Kerr effect**

Accomplishments:

- **Fabrication of nanomagnet sample with size variation**
- **Far-field measurement of magnetization reversal of 250nm nanomagnets**
- **Near field measurement of 100nm nanomagnet**

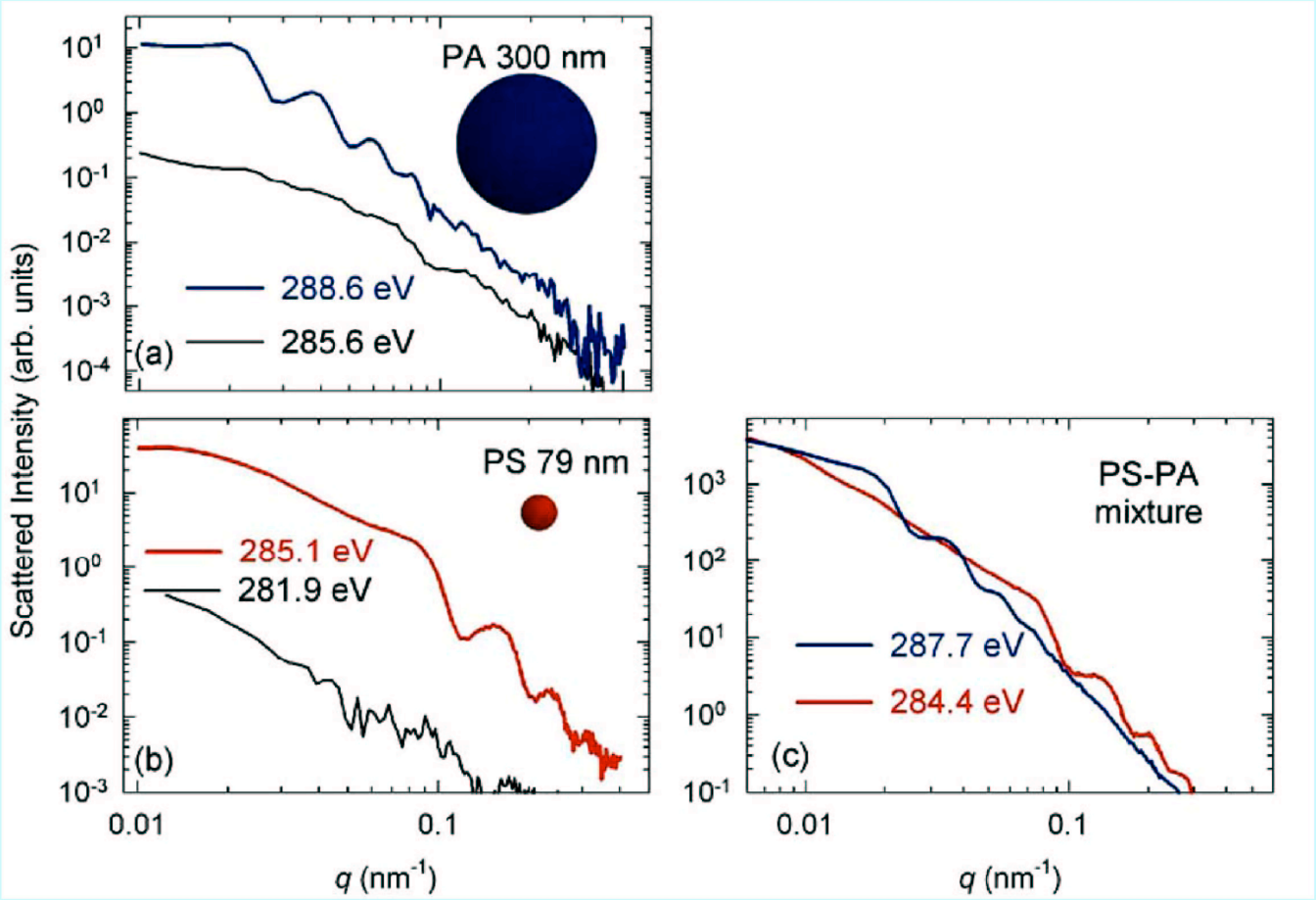


Phase Behavior of a Block Copolymer



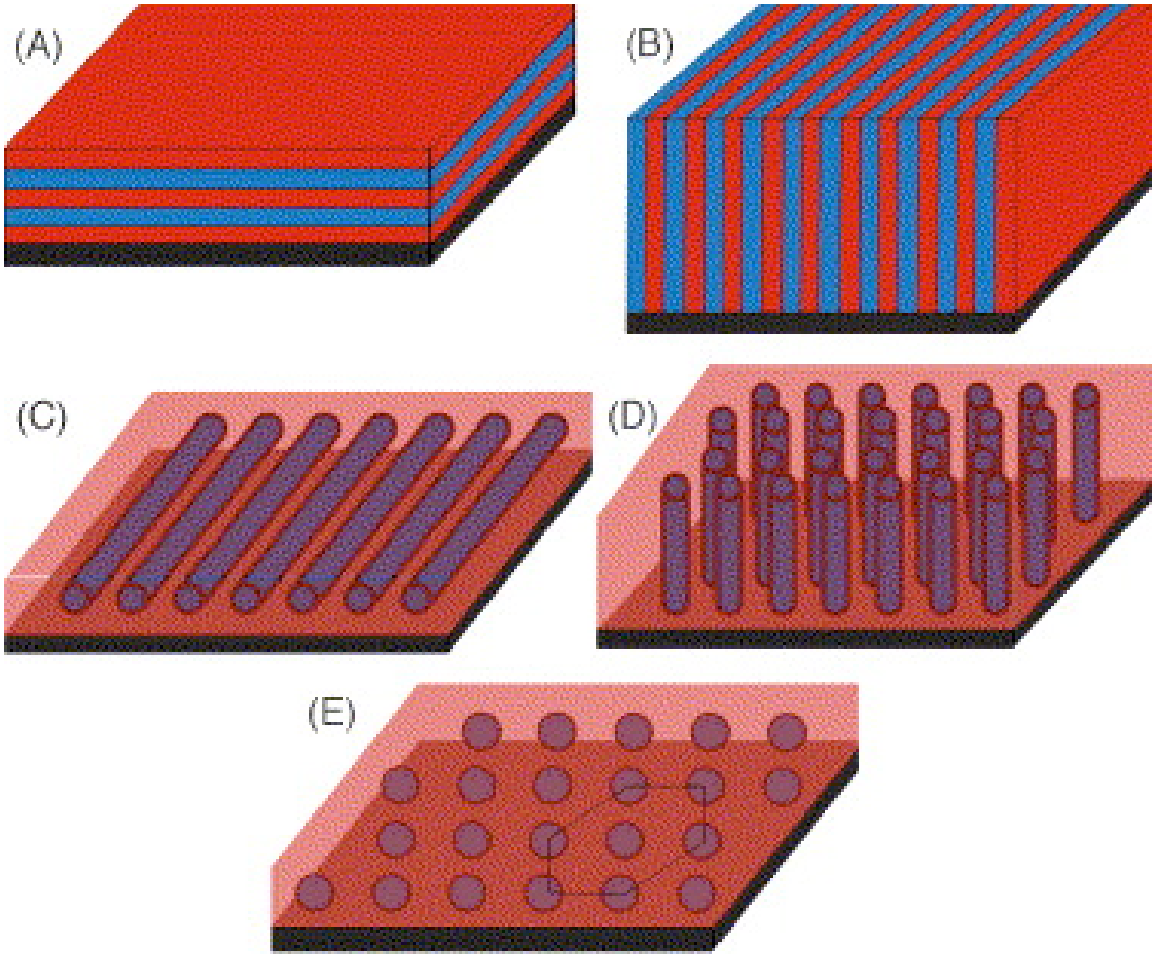
R. Segalman, UCB

Scattering Patterns
(Angle Scans)



G. Mitchell, Dow

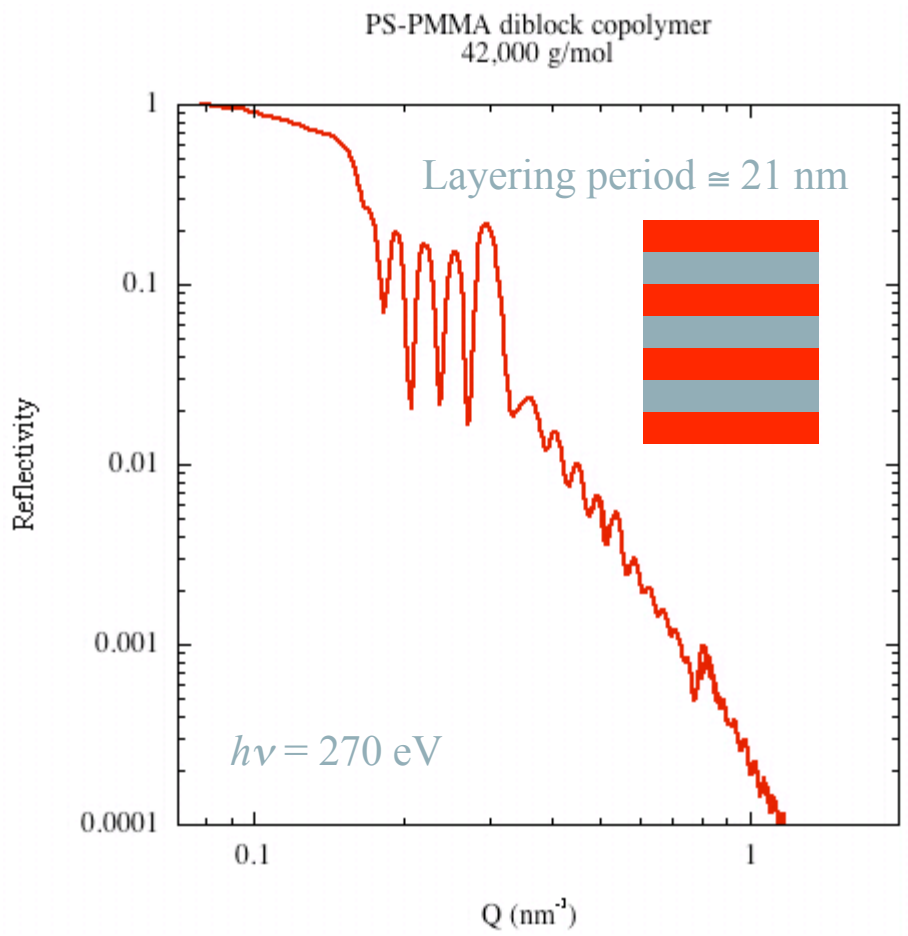
Block Copolymer Thin Films



- Film orientation depends on the interaction of block copolymer with substrate and air interfaces.
- If interactions of A and B with substrate/air are equal, structures perpendicular to substrate *tend* to form.
- If local regions have strong interactions with A/B, perpendicular and *aligned* structures can form.

R.A. Segalman, *Materials Science and Engineering R*, **48** 191 (2005)

Depth-resolved information from diblock copolymer films



Layered phase separation evident from interference

Analysis will provide laterally averaged density profile:

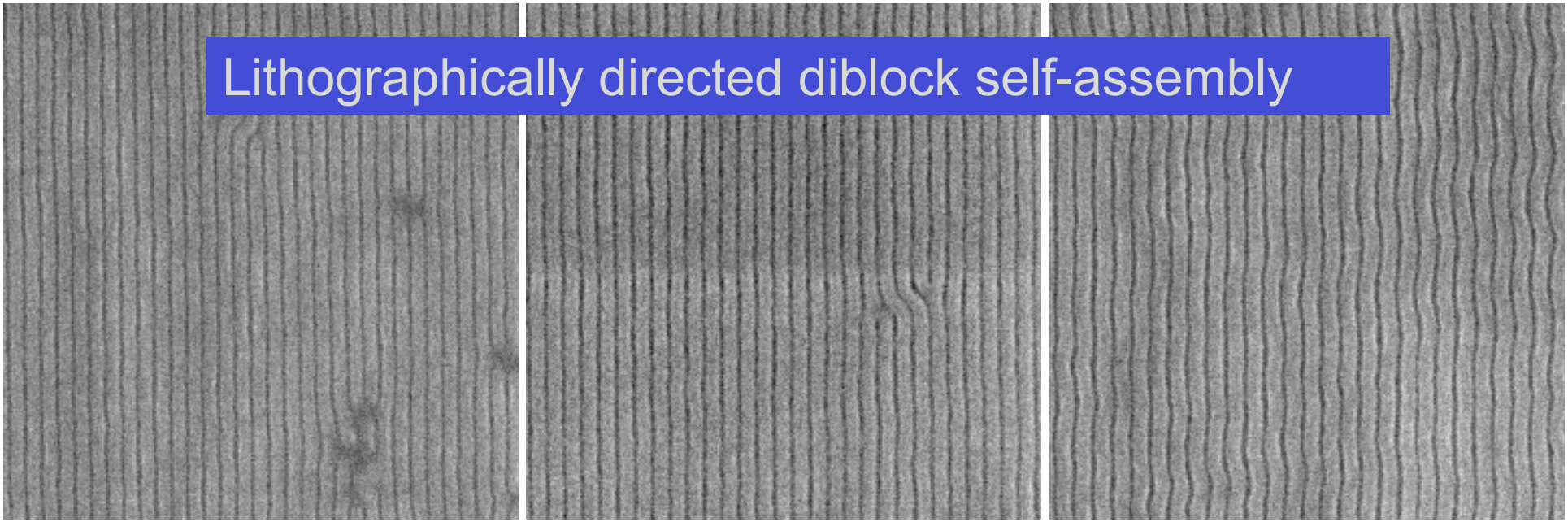
- layer thicknesses
- interdiffusion/roughness
- identity of surface and interface wetting phase

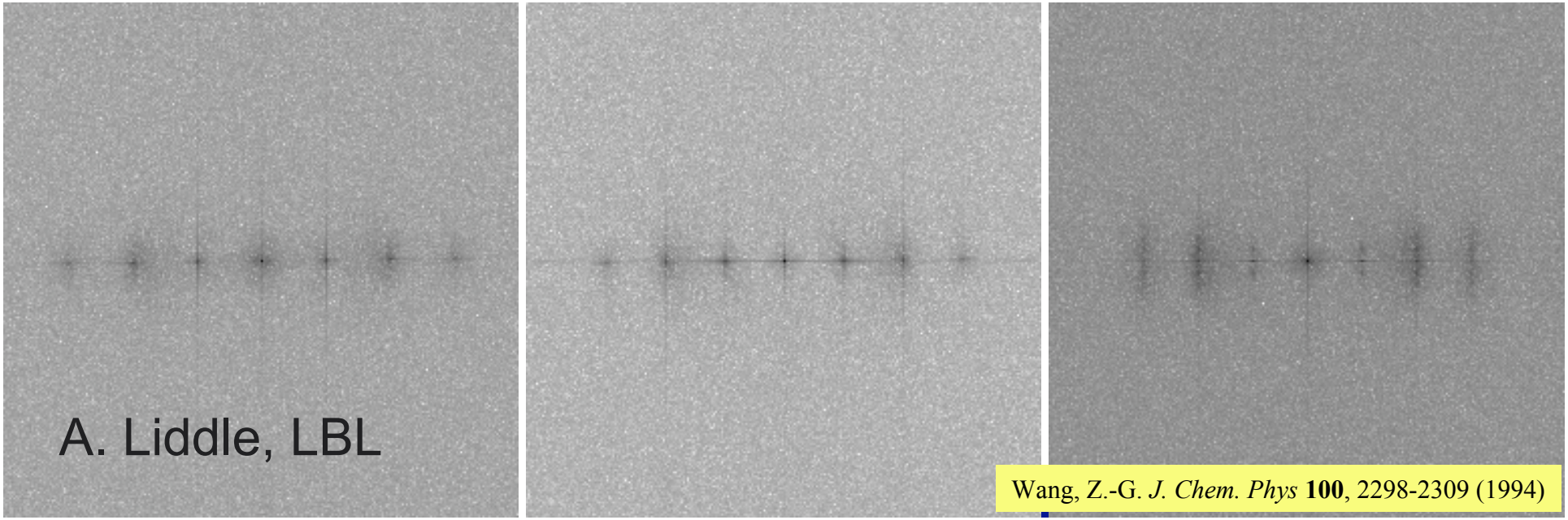
Extensions to:

- more complicated composites, chemical templating
- *in-situ* studies of diffusion, ordering, processing, …

Preliminary study by R. Hjelm (LANL) & J. Kortright

Lithographically directed diblock self-assembly



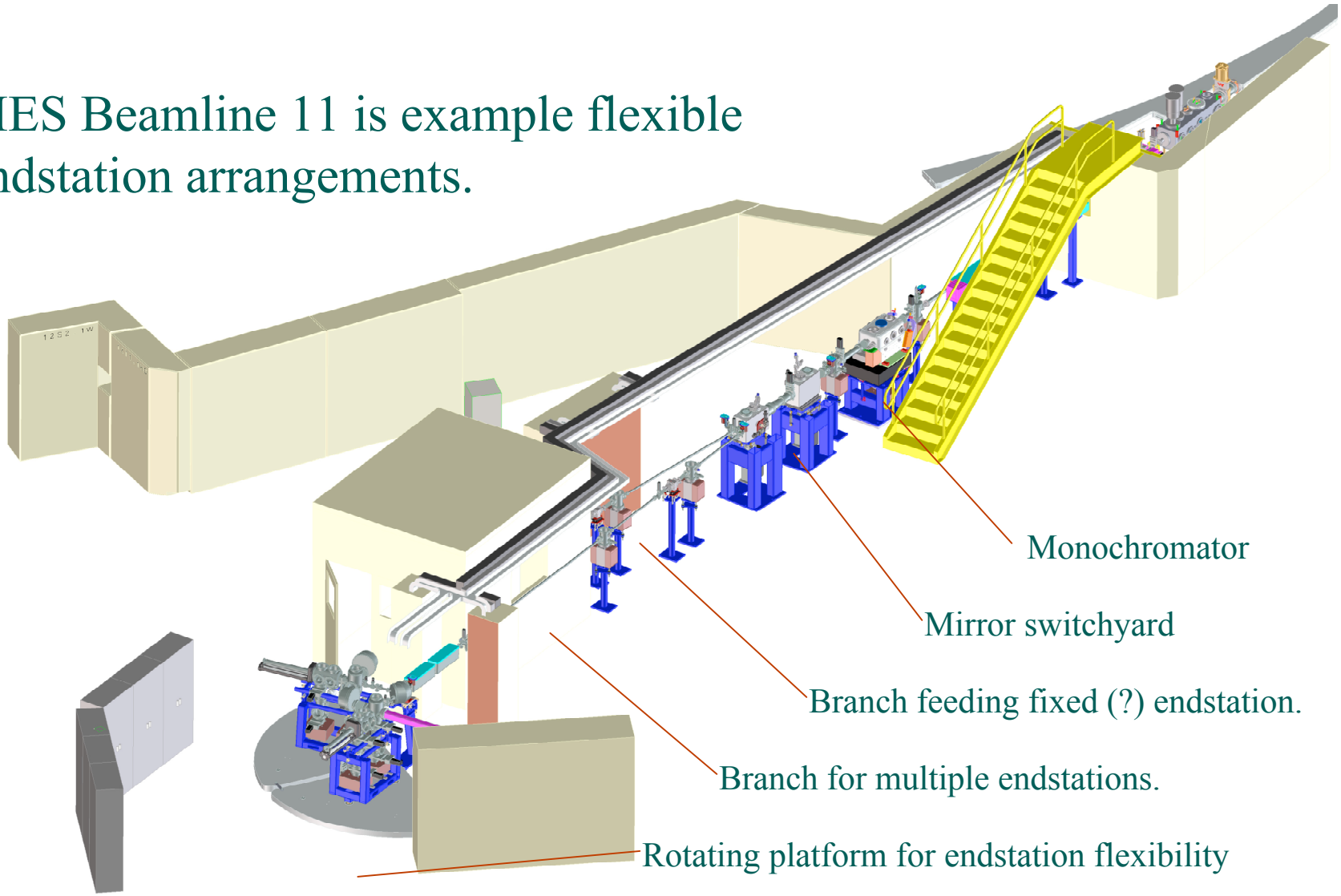


A. Liddle, LBL

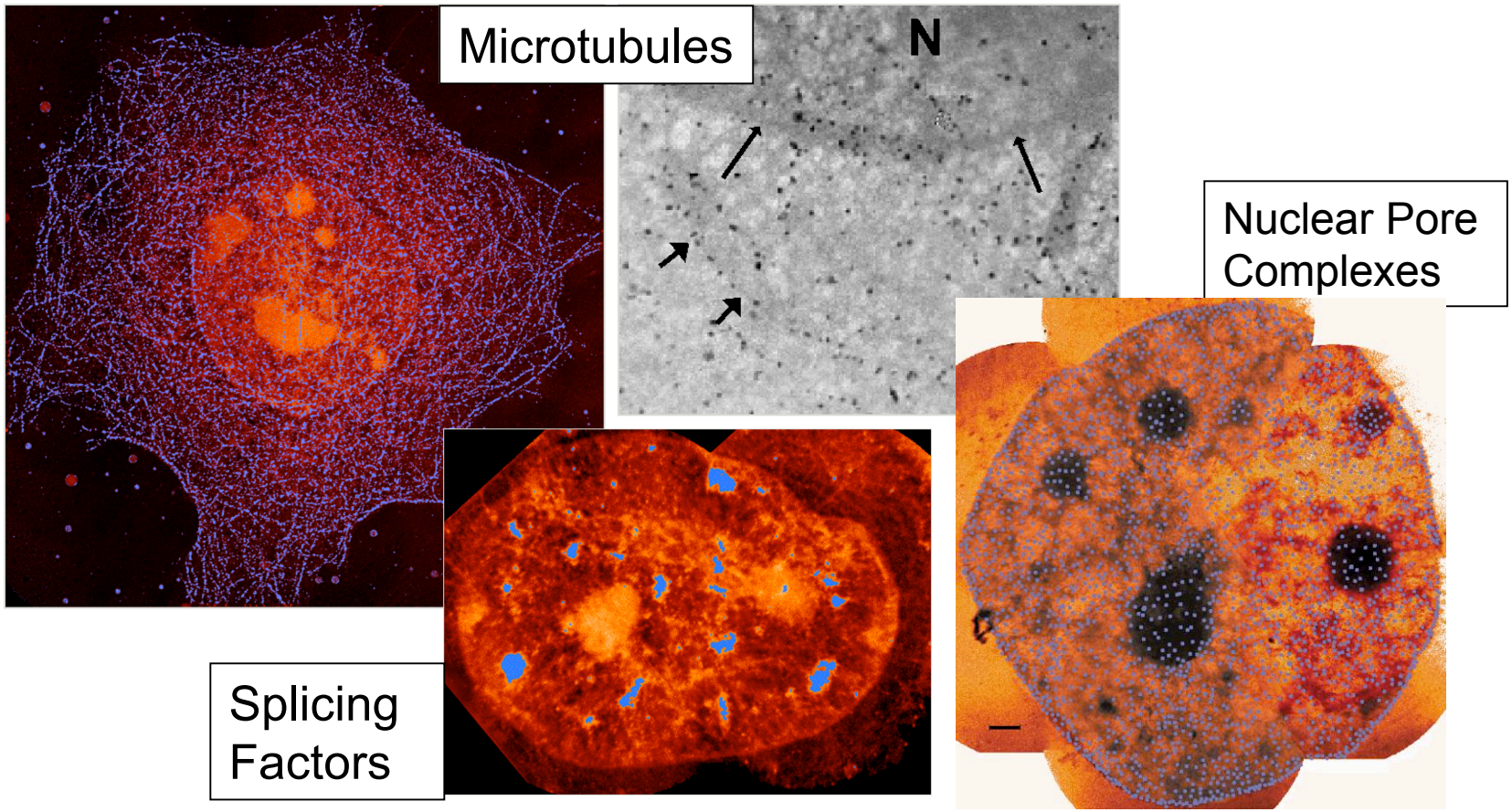
Wang, Z.-G. *J. Chem. Phys* **100**, 2298-2309 (1994)

General beamline plan: chicane long undulator into two short EPUs, one for scattering

MES Beamline 11 is example flexible endstation arrangements.



Immunolabeling for X-ray microscopy - Gold labeling



Although Au works well for X-ray microscopy, it is not possible to perform double or triple labeling with such probes.

C. Larabell, UCSF

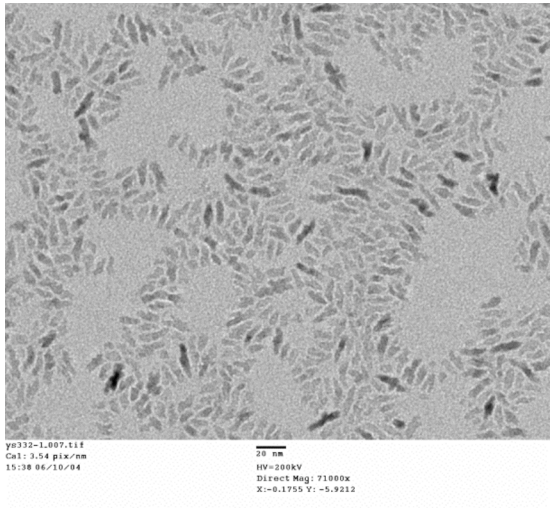
Nanoparticles as Novel Soft X-ray Probes

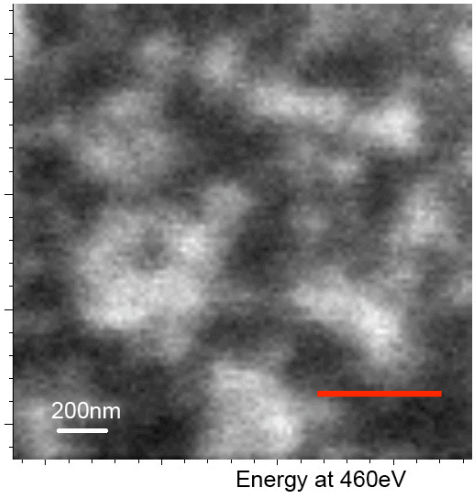
- Ti L shell x-ray absorption lines (~463 eV) falls into the 'water window' region of soft X-ray microscopy.

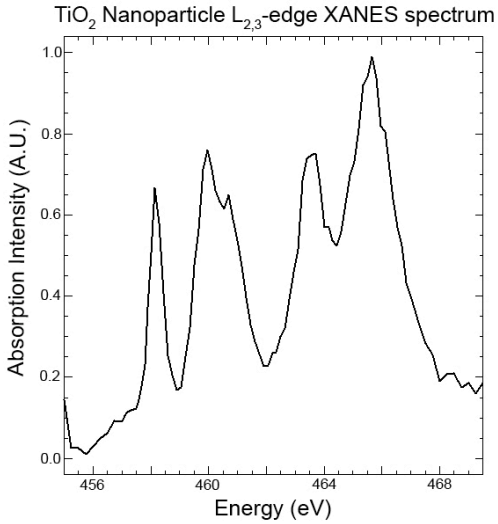
- TiO_2 label is easily distinguishable from another label such as nanogold.

- Double labeling
  - gold-tagged antibody probes to label low abundance proteins
  - TiO_2 nanoparticle to label more abundant proteins such as cytoskeletal networks (actin, tubulin)

Preliminary STXM Studies of TiO_2 Nanoparticles







TEM STXM XANES

- TiO_2 nanoparticles (5 nm x 20 nm) dispersed on silicon nitride membrane (TEM sample)

Y. Yin, TMF

Ag-Au Hollow Nanospheres: What questions can ALS answer?

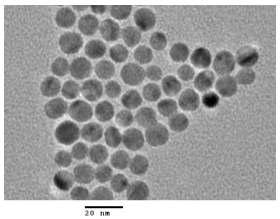
XAS:

Mixing of Au, Ag layers?
Vibrations in nanostructures - what's different between sphere and shell?

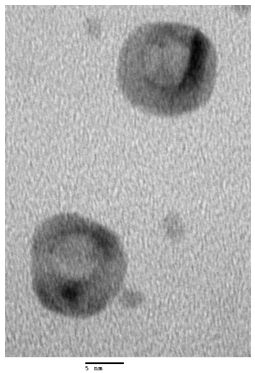
XPS:

Are there ligands on the inside as well as outside?
What are the plasmons like?
Is the shell electronically like a thin film?

solid Ag spheres



Au^{3+}



hollow Au-Ag shells

Image courtesy of Y.D. Yin - Molecular Foundry

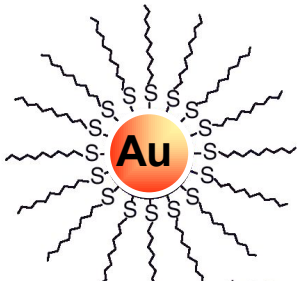
WAXS:

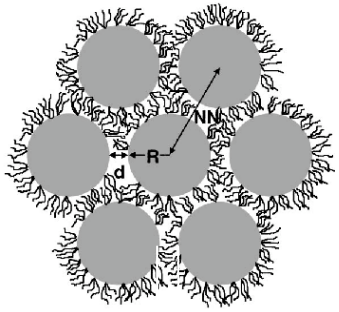
Is the shell a single crystal? What's the grain size?
Is it single-phase? Graded lattice spacing?
Strain vs. pressure?

SAXS:

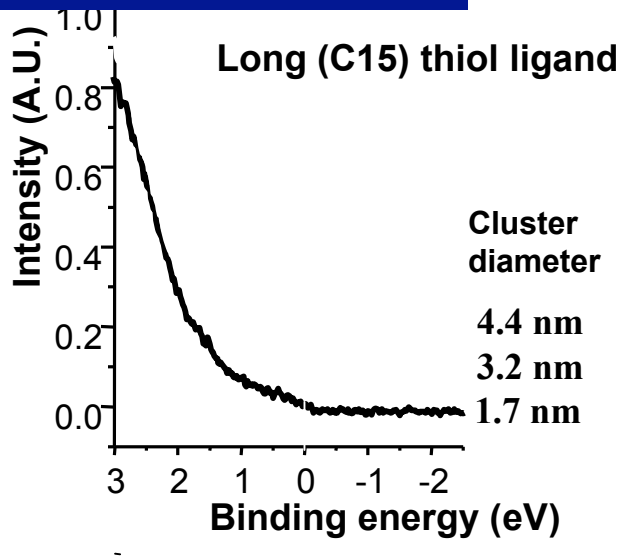
Time dep. of inner, outer diameter.
Does the pore start on-center?
Does Au form a shell before replacing Ag?

Size and distance dependent Fermi level structure of thiol-stabilized Au Nanoparticles



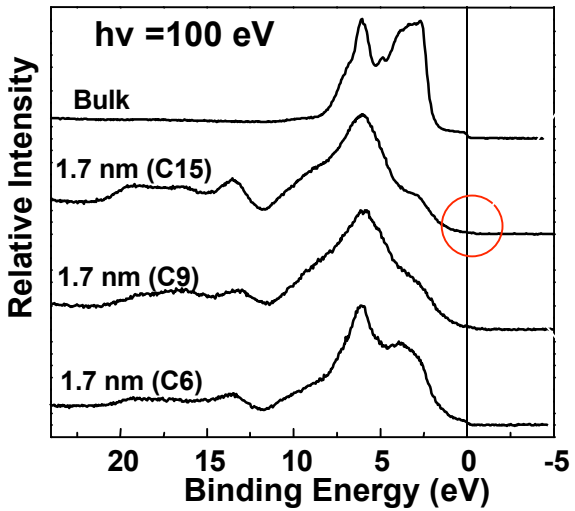


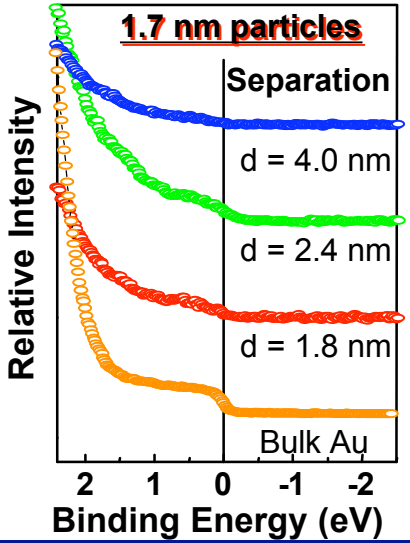
d

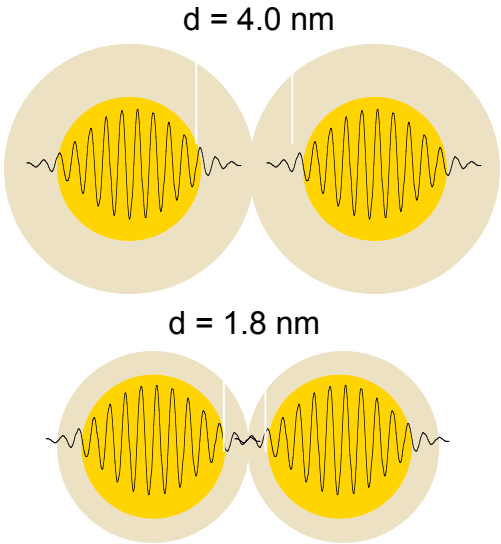


Fermi level density reduction due to Coulomb Blockade effects: $U_c = e^2/2C$, $C = 4\pi\varepsilon_o\varepsilon r$

Cross-coupling (tunneling) when particles are close restores density of states at Fermi level







Hongjina Liu et al. / MSD-LBNL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Ask not what the ALS can do for the Foundry…
Ask what the Foundry can do for the ALS!
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