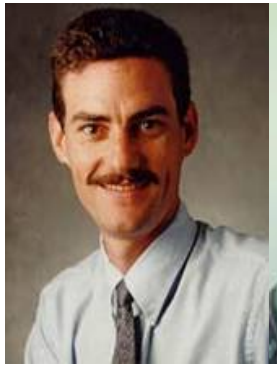
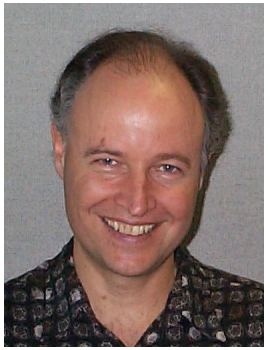
MSU Center of Research Excellence in Complex Materials (CORE-CM), established Fall 2009

CORE-CM develops teams across CNS, Engineering and Nano-Medicine

Center mission

The CORE-CM mission is to promote excellence in materials research on the MSU campus through high quality multidisciplinary group research, infrastructure development, training programs and technological innovation.

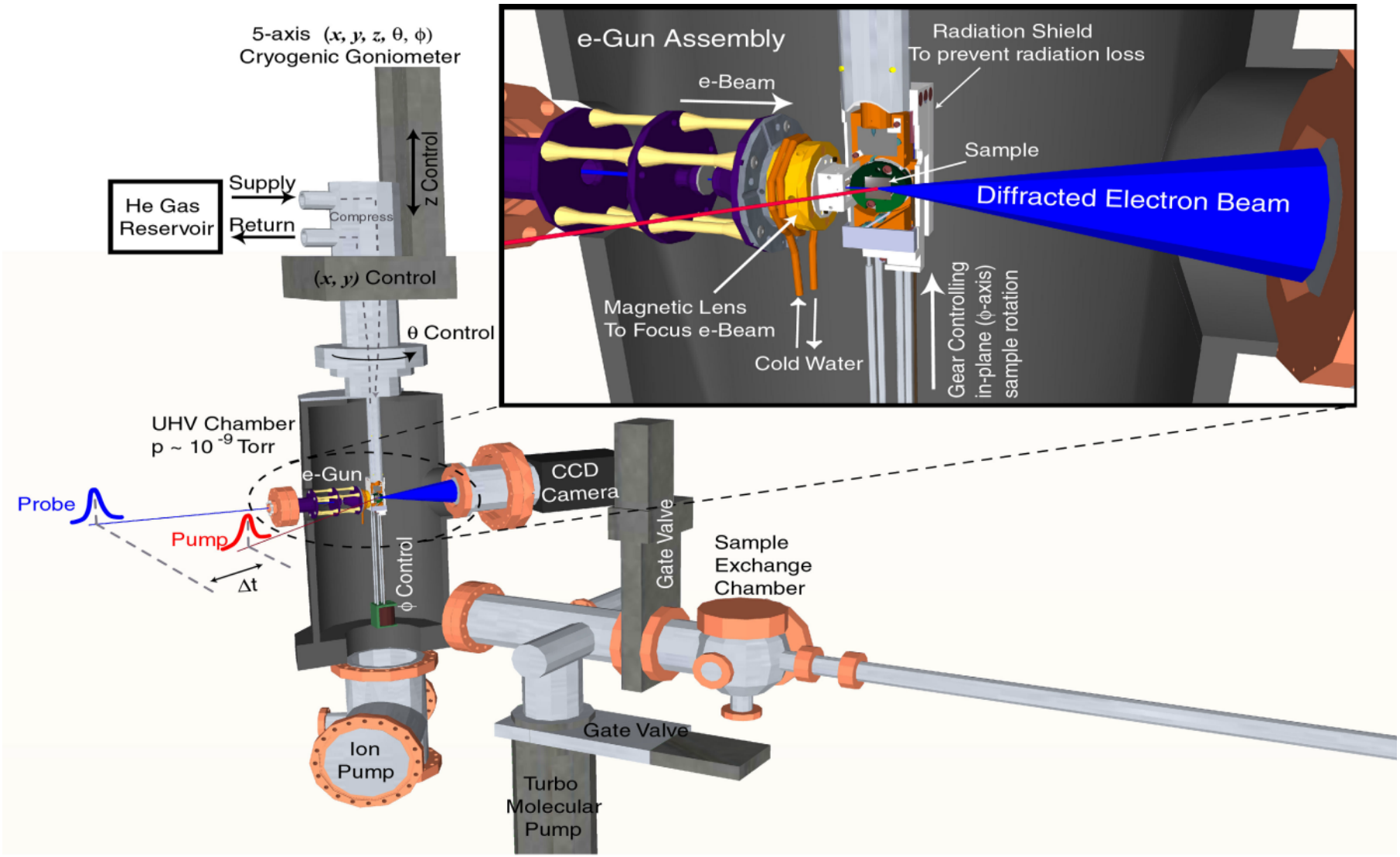




Developing groups competitive for federal group and center calls, along with shared infra-structure projects are primary goals. Both academic and industry based groups are promoted.

Some Research Groups (lead faculty):

Thermoelectric materials (Morelli)
Organic solar (Lunt, McCusker)
Nanotoxicology (Worden)
Ultrafast diffraction (Ruan)
Battery materials (Drzal)
Fuel cells (Barton, Reguera, Promislow)
Materials in extreme environments (Bollen)

Ruan - Designing and building the worlds fastest e-microsope

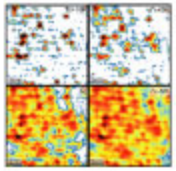


Other members of microscope MRI development team: (Berz, Crimp, Duxbury)
Also affiliated with NSCL/FRIB materials groups

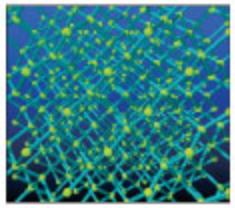
New Frontiers in Sciences Enabled by fs-EM

Imaging Material Transformation

Phase transition of high temperature superconductor

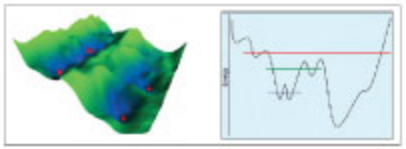


Electron holography of superconductor (Lichte, Tonomura)



Graphite to diamond transition through photoexcitation
(Ruan, Tomanek, Drzal, MSU)

Imaging Molecular Function



Free energy landscape of molecules

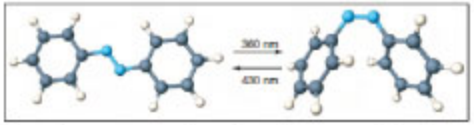
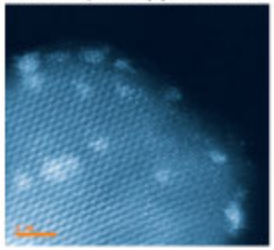


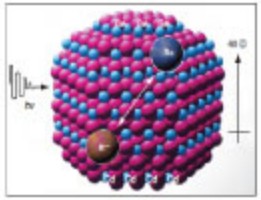
Photo-interconversion of two isomers of azobenzene
(Barret, McGill)

Au Nanocatalyst Supported on TiO2 ...

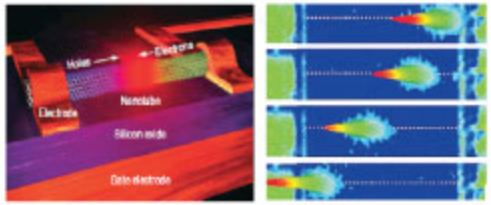


(Zilin Wu, ORNL
Landman, Georgia Tech)

Imaging Electron Dynamics

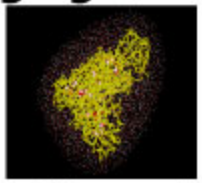


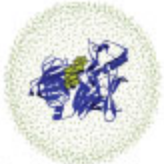
Photovoltaic processes in nanoparticle (Kilmov, LANL)



Carrier dynamcis is quantum nanostructures
(Kim, Culombia; McEuen, Cornell..)

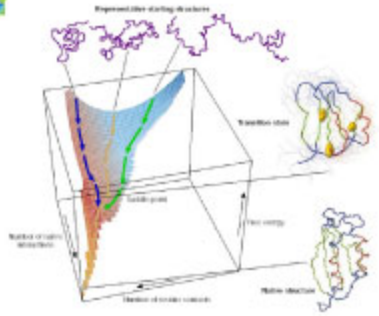
Imaging Biological Function





Solvated protein in nanocavity (water) ... (H. Grubmuller, Max Planck Inst.)

Protein folding dynamics
(Dobson, Cambridge)



Key areas

High-Tc superconductor

Laser machining

Water splitting

Photo-catalysis

Nano-electronics

Photo-voltaics

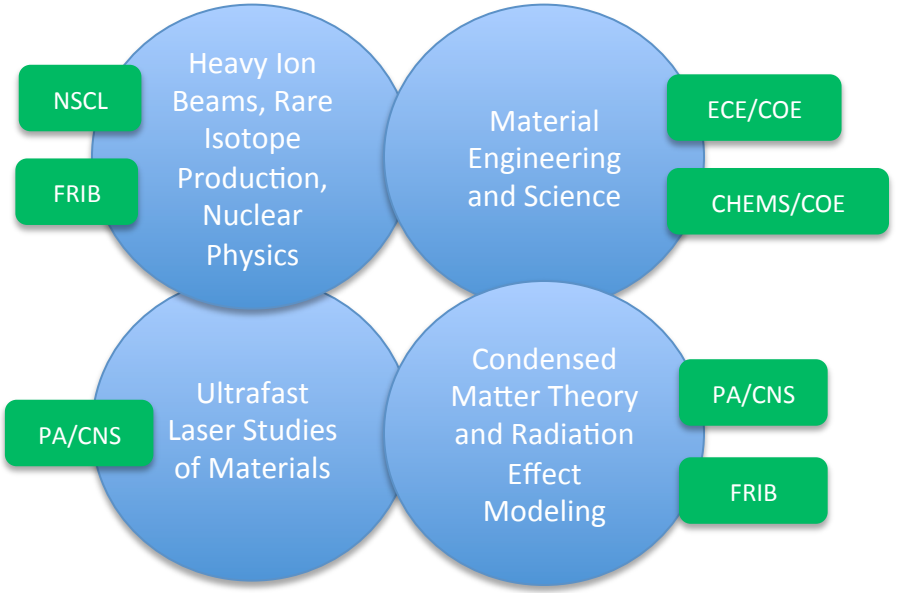
Protein-folding

Drug discovery

FRIB/NSCL – CORE-CM materials group (SPG)

Leverage unique MSU expertise and capabilities to address extreme materials problems of critical local and national importance

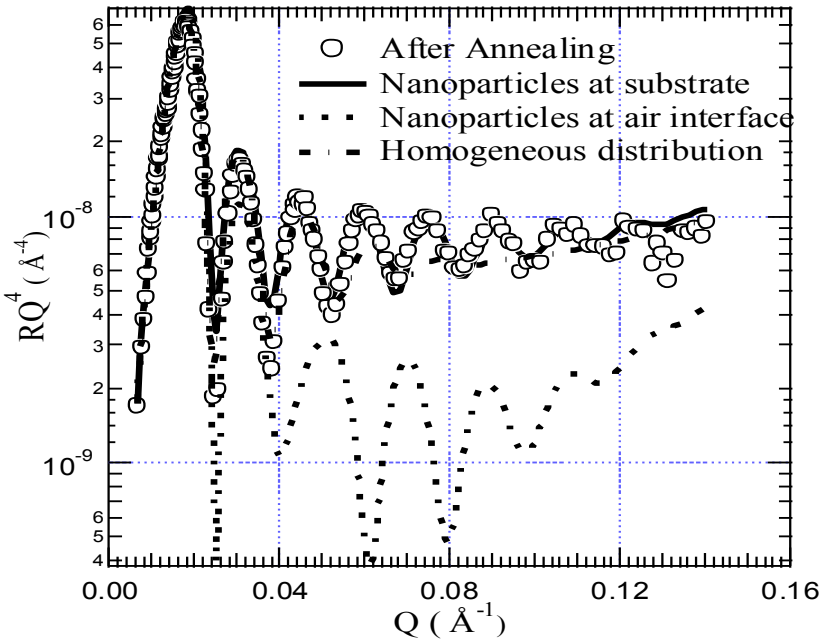
- **Develop and study key materials** under extreme radiation, stress, temperature conditions (Graphite, Diamond, Ti alloys)
- **Develop a broad MSU team** to leverage NSCL (and future FRIB) beam conditions and MSU's expertise in material science and engineering



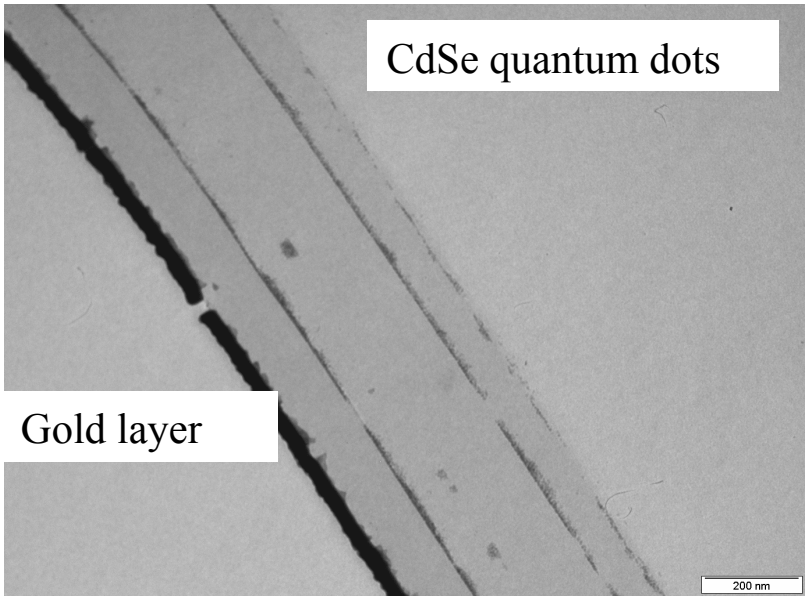
- **Physics and Astronomy** (**Duxbury, Ruan**)
- **Electrical and Computer Engineering** (**Grotjohn**)
- **Chemical Engineering and Material Science** (**Boehlert**)
- **National Superconducting Cyclotron Laboratory** (**Mittig, Stolz**)
- **Facility for Rare Isotope Beams** (**Bollen, Pellemoine, Ronningen**)

Use swift heavy ions to for nanolithography and to create nanostructured materials

Segregation of nanoparticles to polymer thin film surfaces and interfaces



Neutron reflectivity of PS NP in PS – Segregation to substrate due to entropy



TEM functionalized CdSe quantum dots in PS – NPs segregate to free surfaces due to dispersion forces

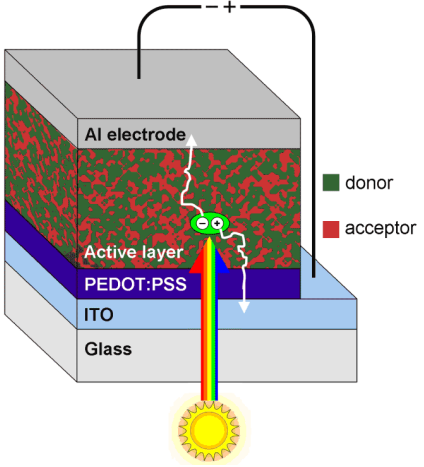
Physical interactions which control nanoparticle segregation

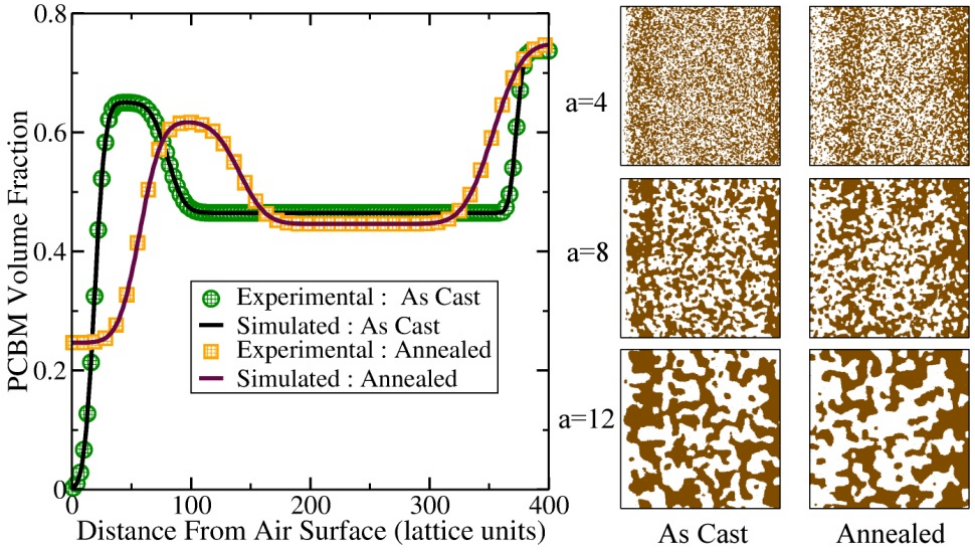
- Entropy is gained when nano-particles segregate to surfaces – e.g. relaxation of polymer confinement at hard substrate.
- Long range dispersion forces play a key role. Systems with similar refractive index have an effective attraction. (monotonic dielectric ordering is favored).
- CdSe nanoparticles have a low n alkane layer at the surface. This leads to an effective dielectric constant which is less than PS (1.59), favoring segregation to the air/PS surface.
- CdSe with Pyridine coating anneal to a SiO_2 (4nm) on Si substrate.

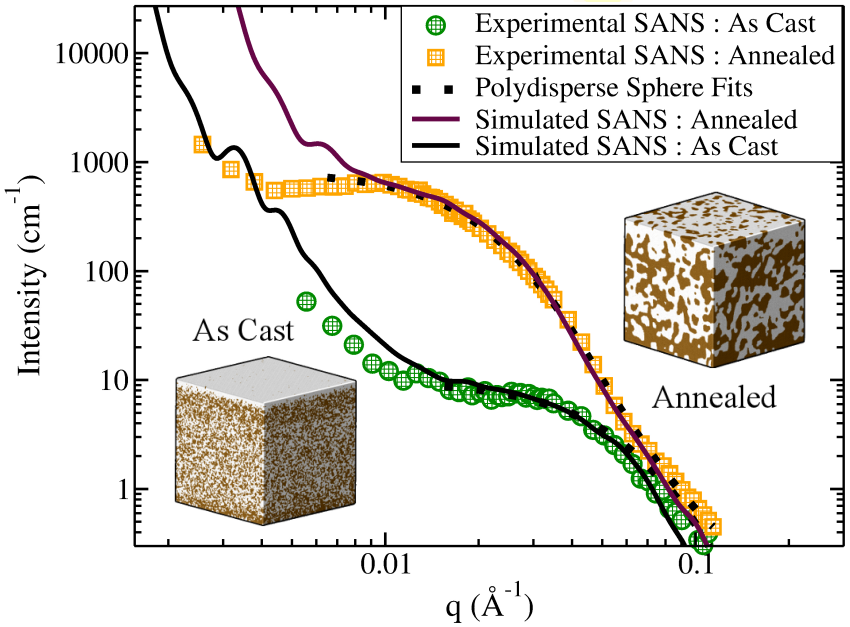
Characterization of NP-Polymer morphology

-NP concentration profile: Reflectometry

-Characteristic domain size: SANS







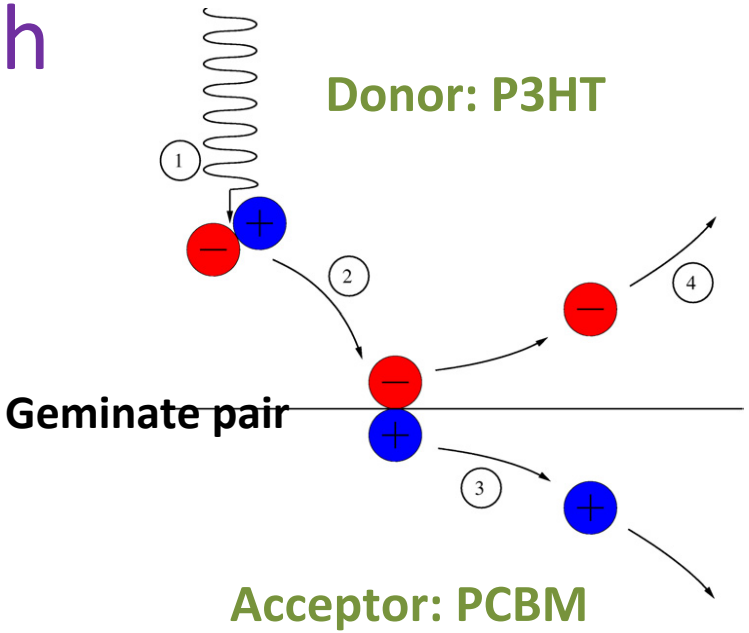
Kiel et al., Nanoparticle agglomeration…., PRL 2011

3-D real space models: Constrained optimization

$$H = -\sum_{ij} J_{ij} S_i S_j + a \int dz |\rho^{ex}(z) - \rho^{m}(z)| + b|p_m - p_{ex}|$$

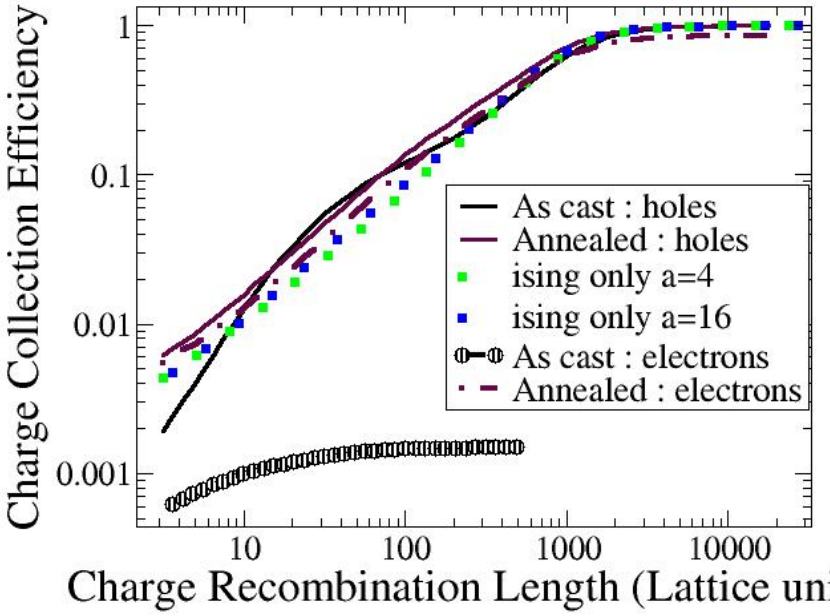
Olds and Duxbury, Percolating bulk heterostructures…., PRE 2012

Dynamic Monte Carlo with First Reaction Method



In our simulations:

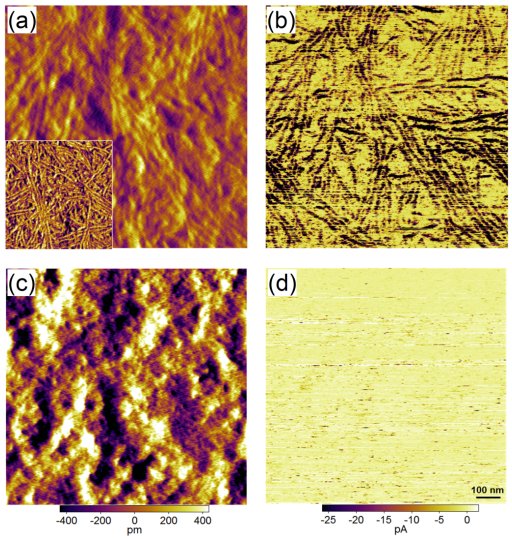
- Excitons are generated uniformly in P3HT at a rate extracted from experiment and diffuse until they dissociate or decay (exciton decay length).
- When excitons find a donor/ acceptor interface before decaying, they form a geminate pair
- Geminate pairs diffuse on the interface until they recombine or dissociate into free carriers hole (pair recombination length).
- Free carriers diffuse until they recombine or are collected at an electrode (free carrier recombination length).



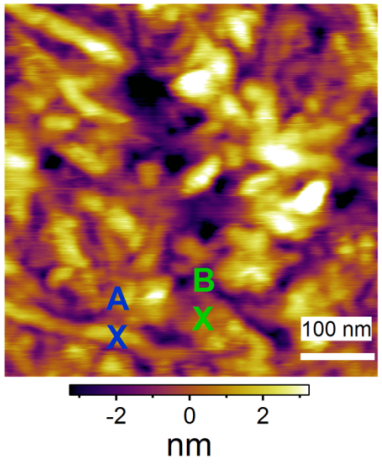
c-AFM hole Injection into fibrous P3HT (J. Sun, P.P. Zhang)

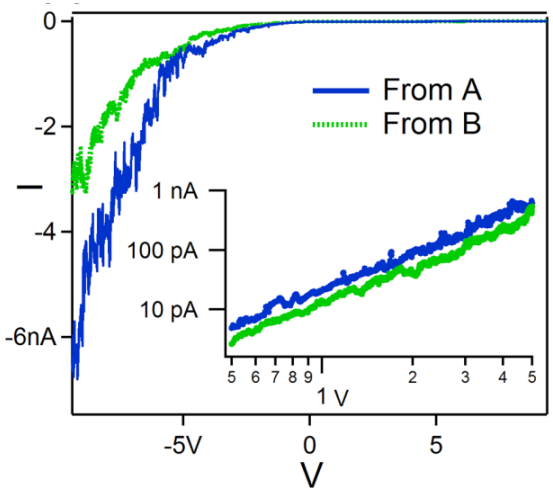
Giridharagopal, Ried,….Ginger,… Nanoletters (e.g. 2012)
Submicrosecond Time Resolution Atomic Force Microscopy for Probing Nanoscale Dynamics

C-AFM images of annealed (a-b) and non-annealed (c-d) P3HT films. (a,c) show the topology, and (b,d) show the corresponding current maps



The c-AFM image showing topography of annealed sample and IV-characteristic at fixed spots A and B





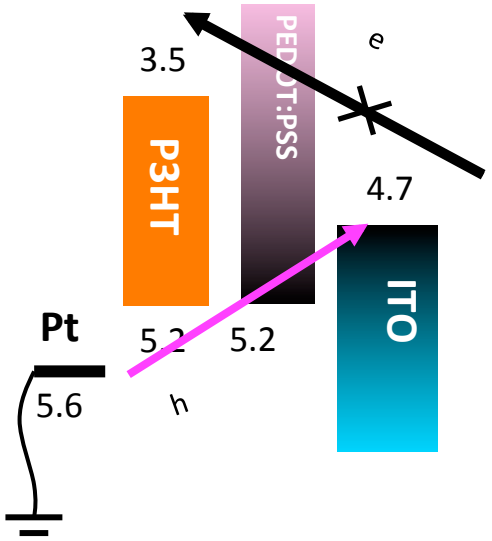
c-AFM current maps and IV relations:

Nanofibers are clearly observed in annealed samples.

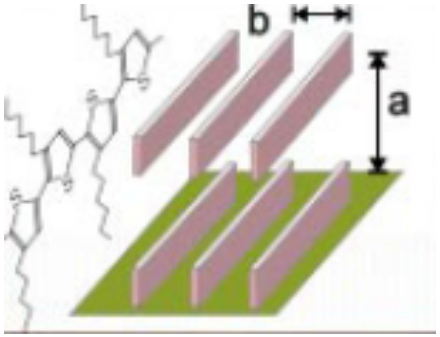
Different currents are measured on and off fiber.

Experimental Result for P3HT (J. Sun. *at. al,* 2012, preprint)

3D Continuum model of Hole Injection System



Hole injection only and anisotropic mobility



H. Sirringhaus et. Al., Nature , Vol 401, 1999

Poisson's Equation

$$\nabla \cdot (\epsilon \nabla \psi) = -q n_p$$

Continuity Equations at steady state

$$\nabla \cdot J_p = 0$$

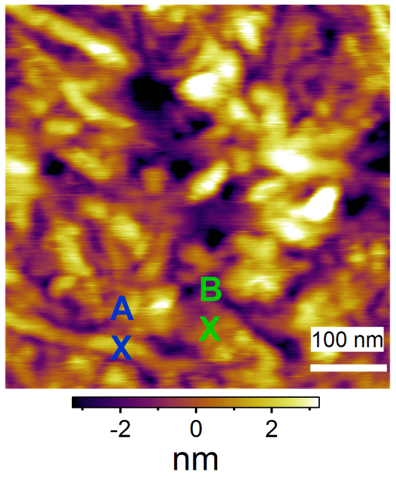
Drift-Diffusion Equations

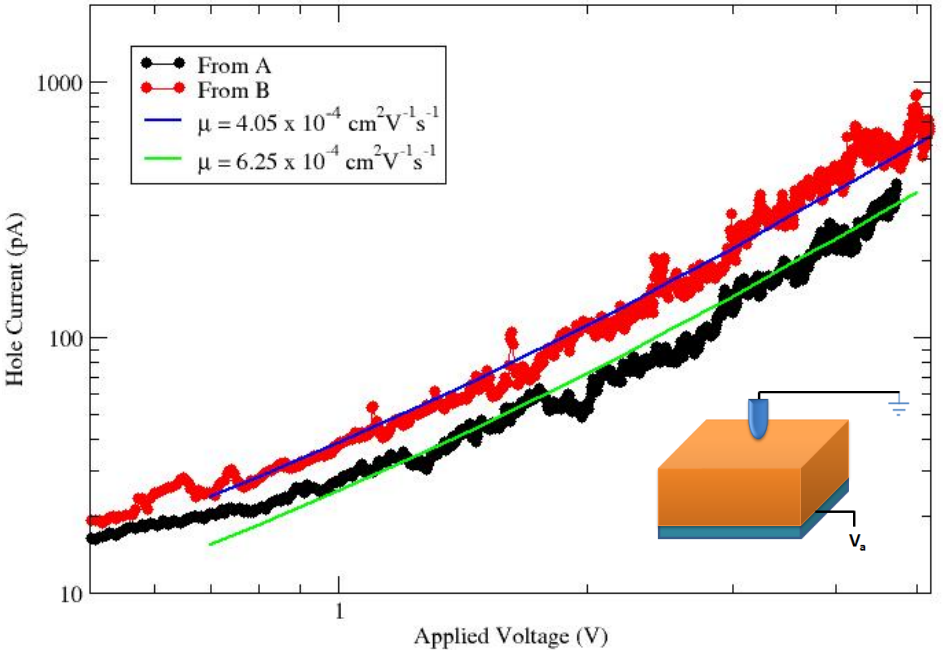
$$J_{p,\zeta} = -q n_p \mu_{p,\zeta} \frac{\partial \Psi}{\partial \zeta} - q D_{p,\zeta} \frac{\partial n_p}{\partial \zeta}$$

$$\vec{\mu}_p(\vec{r}) = \sum_{\zeta=1}^{3} \mu_{p,\zeta}(\vec{r}) \vec{e}_\zeta \quad \text{where} \quad \zeta = x, y, z$$

Einstein relation of charged particles, $D_{p,\zeta} = \mu_{p,\zeta} \frac{k_b T}{q}$

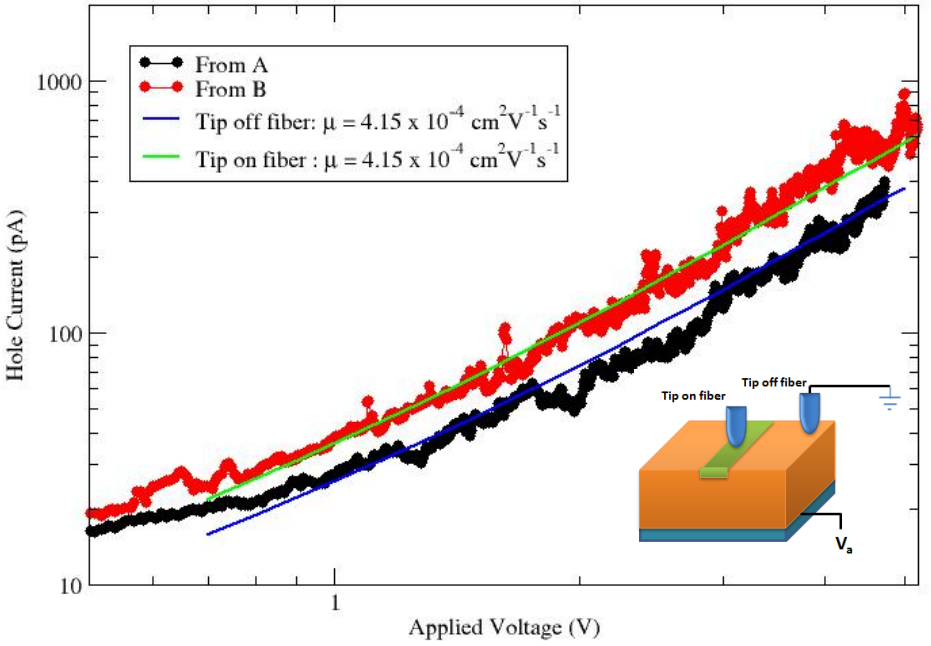
3D Continuum Device Simulation Of Anisotropic Fiber





- Implementing fiber in to the morphology, the experimental result can fit to the same value of back ground hole mobility around

$$\mu_o \approx 4.15 \times 10^{-4} cm^2 V^{-1} s^{-1}$$



MSU group, preprint 2012

Mesoscale Priority Research Direction

Taming complexity from atoms to the mesoscale: NP/organic hybrids

Opportunity

Nanoparticle(NP)/organic hybrids are the basis of many energy harvesting, storage and utilization systems. The functionality of these systems is controlled by NP dispersion and segregation, interface structure, organic cystallinity etc. Taming this complexity through control of synthesis from the atomic to micrometer (A->M) scales, guided by high precision static and dynamic characterization and modeling would be transformative across a broad range of materials systems and devices.

Approach

Direct self-assembly using dispersion forces, entropy and electrostatics toward either equilibrium or strongly metastable structures. Polymer architecture, solvent and/or thermal annealing etc to further control A->M structure. Combine scattering, reflectometry, AFM, SEM, TEM, nano-CT etc with modeling to find percolating 3-D real space A->M models. Use integrated Ab-initio, Kinetic MC, and continuum approaches with A->M model architectures to correlate performance with morphology and hence with synthesis and processing

Meso Challenge

- Synthesis and processing to control A->M structure
- Characterization methods to generate 3-D interconnected A->M models consistent with experimental data.
- Characterization of the dynamics of charge transport across A->M length scales and fs to seconds time scales.
- Modeling of charge generation and reactive transport in experimentally consistent A->M architectures.
-Optimize A->M architectures for applications

Impact

Success in multiscale synthesis, integrated A->M characterization and multiscale modeling would open many new opportunities for materials and device optimization. NP/organic hybrids are a good place to start as they have a broad knowledge base, they exhibit a wide range of novel physical and chemical phenomena, and they are of interest for a broad range of energy and other applications.

Contact: Phil Duxbury, MSU

A. Balazs, T. Emrick, T.P. Russell, Nanoparticle polymer composites: where two small worlds meet, Science 314, 5802 (2006)
M.E. Mackay et al. General Strategies for NP dispersion, Science 311, 1740 (2006)
S.R. Forrest, The path to ubiquitous and low cost organic electronic devices on plastic, Nature 428, 911 (2004)
M.C. Dennler, G. Scharber, C.J. Brabec, Polymer-Fullerene Bulk heterostruture solar cells, Advanced Materials, 21, 1232 (2009)
D. deLongChamp et al, Molecular characterization of organic electronic films, Advanced Materials 23, 319 (2011)