
Materials Science Division

Meeting

June 3, 2005

New Program and FWP: Hoydoo You et al
Electrocatalysis of the Oxygen Reduction Reaction

DOE review January 25-28

Management Review April 6

BES Funding

Raises and Bonuses

Strategic Paths

News Updates

New FWP: BES Hydrogen Initiative

Fundamental Studies of Electrocatalysis for Low Temperature Fuel Cell Cathodes

Hoydoo You (Coordinator)

Nenad Markovic, Goran Karapetrov, Zoltan Nagy,
Peter Zapol (MSD/CHM/CNM), Debbie Myers (CMT),
Yuri Tolmachev (Chemistry, Kent State U)
Woods Halley (Physics, U Minnesota)

new FWP team

- coordinated research
 - science management
 - budget management
- \$760K/yr*

*reception for the team
after meeting*

New FWP: Electrocatalysis Science

measurements

in situ x-ray structure and spectroscopy APS
SPM in catalytic environments
electrochemical characterization
theory and modeling

systems

single crystal surfaces
nano-patterned surfaces
nanoparticle catalysts
real fuel cell catalysts

DOE Review of CMP, MC

January 25-28, 2005

review strategy

simple message delivered 3 times: review doc, oral talks, posters

message: future, accomplishments, synergy

energetic world class science

feedback

reviewers: establish collaboration, arrange visits

BES: all smiles, "flawless review," "no issues"

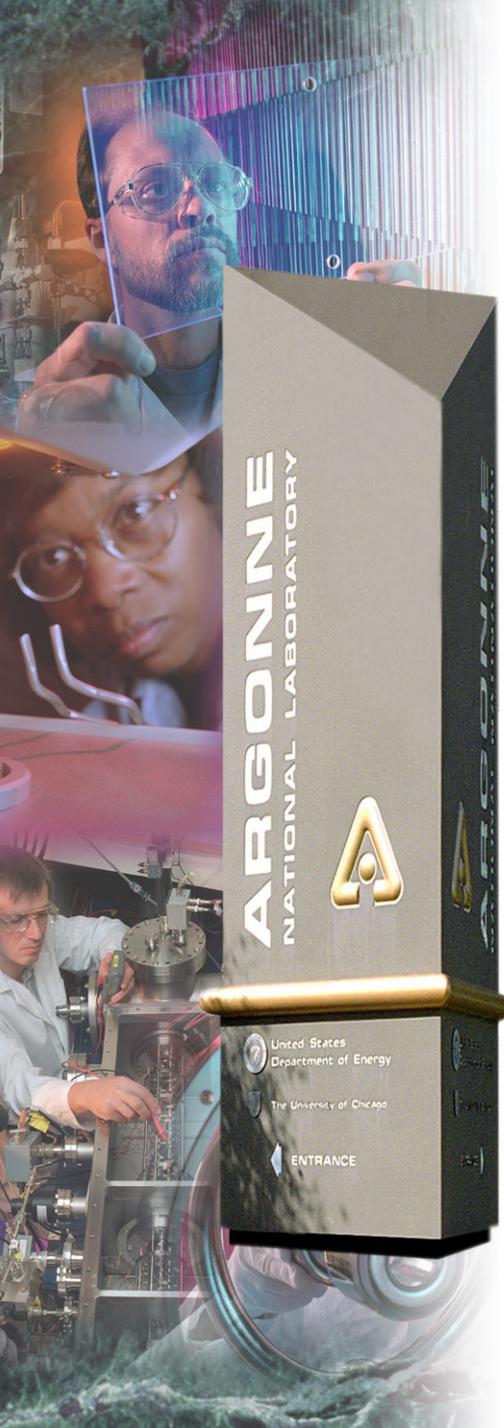
Thanks to all!

Ulrich Welp, Paul Fuoss, Urs Geiser

Marlene Metz, Suzanne Marik, Dave Lehman

FWP leaders, speakers, poster teams

administrative and technical support staff



Materials Science Division Management Review

George Crabtree

Mike Pellin

Sam Bader

Dean Miller

April 6, 2005

Argonne National Laboratory



*A U.S. Department of Energy
Office of Science Laboratory
Operated by The University of Chicago*



Mission

Create and Deliver World-Class Science
to the International Community

Create
Explore
Understand

Focus: Energy

Energy is society's dominant problem

Materials are key to its solution

World-Class Science ⇔ *Engaged People*

teams activate tasks
evaluate equipment proposals
organize reviews/workshops
create white papers/proposals
seminars/colloquia/nanolunch

...

reformulate for each task
independent of FWP structure



*MSD strategic planning workshop
March 2004*

Approach

Integrate: synthesis, characterization, theory, simulation

Innovate: science-driven instruments and techniques

Explore: new materials of increasing complexity

Interact: critical mass of people, ideas, and techniques

Scientific Opportunities

Synthesis: enabling world-class science

Emergent behavior: interacting degrees of freedom

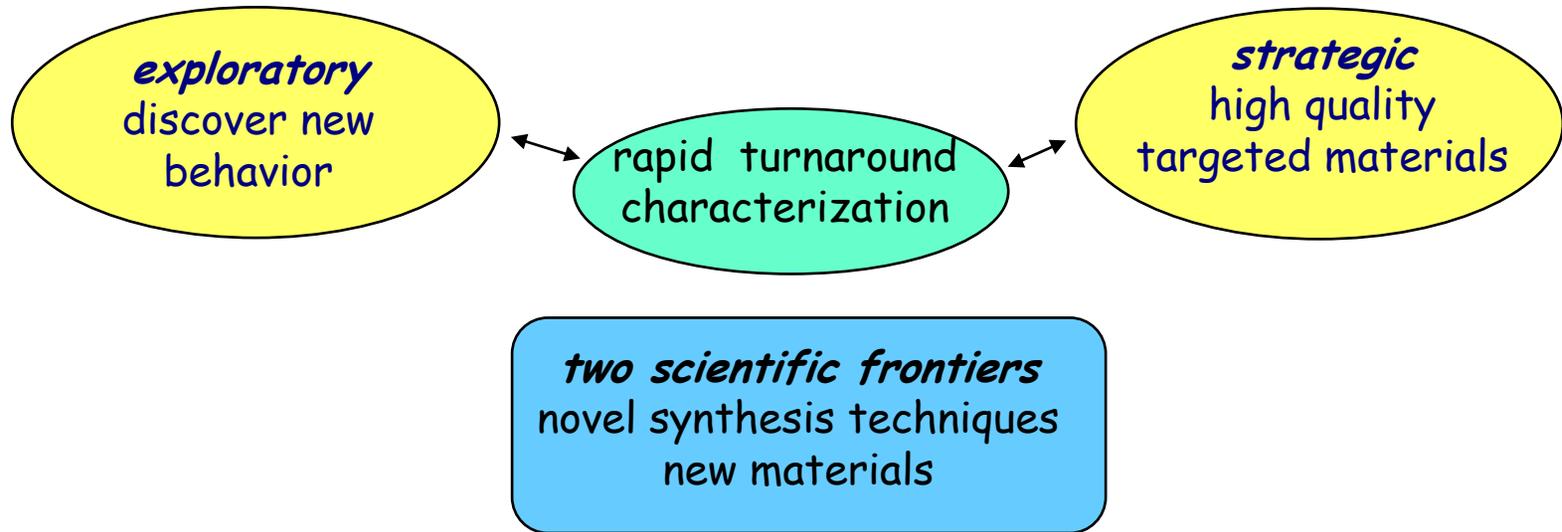
In-situ characterization: watch dynamics in real time

New materials

interacting components, asymmetric structure,
competing order, coupled responses . . .

Physical behavior on the nanoscale

Opportunity: Synthesis



- bulk: high pressure new structures, extended doping ranges, exotic oxidation states
- artificial layers: ALD, digital alloys \Rightarrow control stacking with unit precision
- self-assembled nanostructures: colloidal drop-casting, kinetic electrodeposition, bio-scaffold assembly

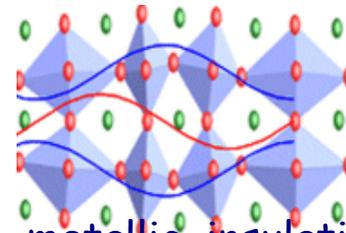
John Mitchell, Paul Canfield, John Sarrao, Doon Gibbs, David Mandrus
Materials Synthesis Network

Opportunity: Emergent Behavior

Complex oxides

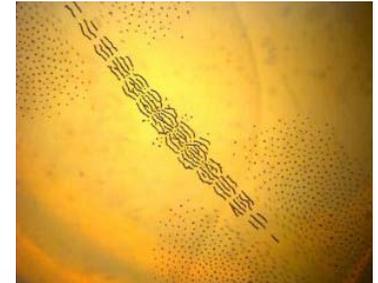
spin, charge, lattice interactions

ferromagnetic, ferroelectric, superconducting, metallic, insulating
complex disorder

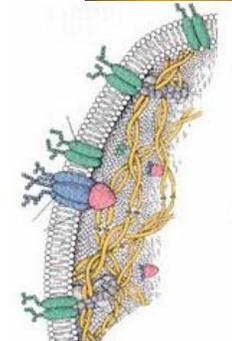


Electromagnetically self-assembled granular matter

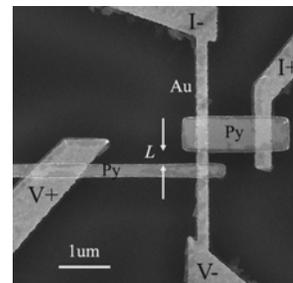
competing long/short range interactions



Biomolecules/nanoparticles in artificial hosts



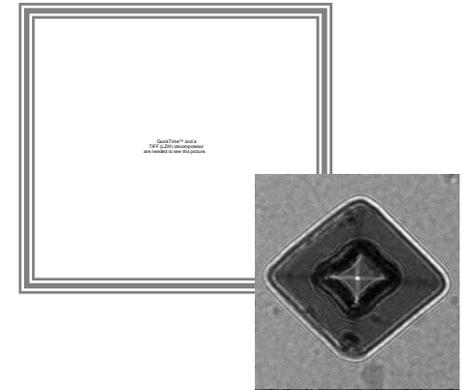
Decoupled spin-charge systems



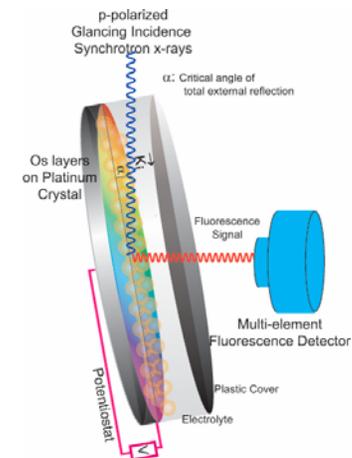
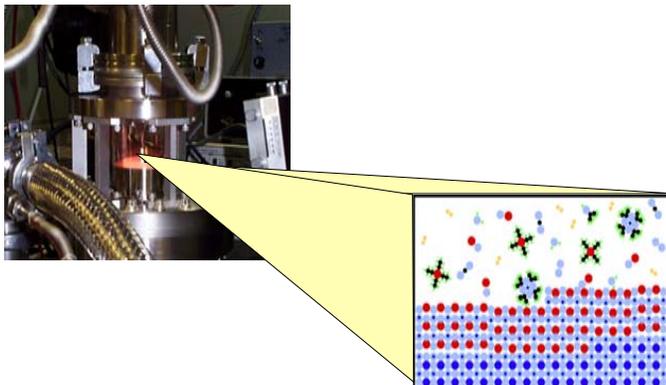
Opportunity: In Situ Experiments

explore dynamic mechanisms in real time

- polarization reversal
- film growth
- oxidation
- chemical catalysis/reaction



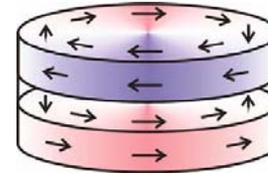
forefront instruments for electron, neutron, photon scattering



Opportunity: Materials of Increasing Complexity

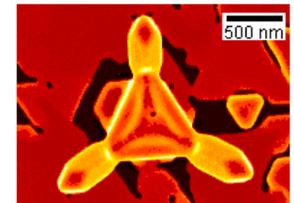
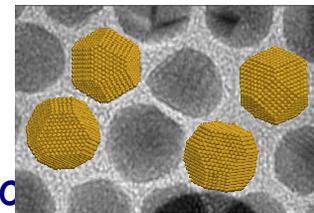
multi-component hybrids

multi-ferroic, bio/inorganic, soft/hard,
magnetic/superconducting, core-shell, core-sheath

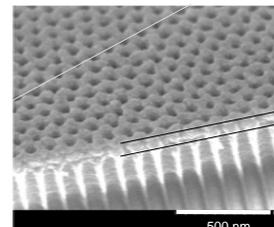


nanoscale assemblies

lithographic structures, bio-scaffolds,
colloidal aggregates, kinetic electrodeposition



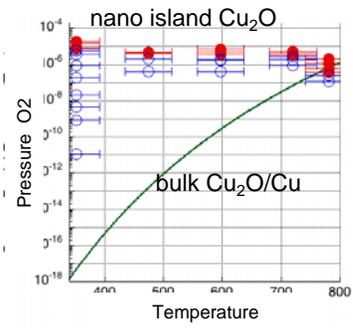
nanoporous materials



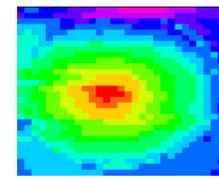
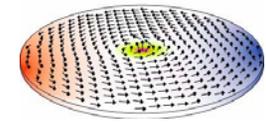
a 101 nm
dia 45 nm
Ag
Nb
AAO

Opportunity: Physical Behavior at the Nanoscale

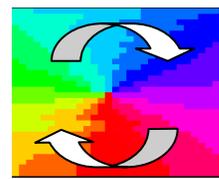
nanoscale surface chemistry



confined magnetic/electric polarization

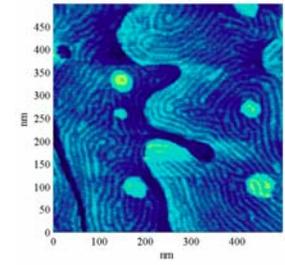


magnetic amplitude

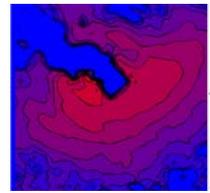


magnetic orientation

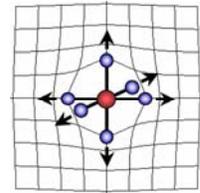
laterally patterned charged and polar surfaces



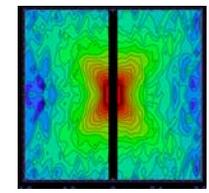
short/medium range order
frustration, complex disorder



electrons



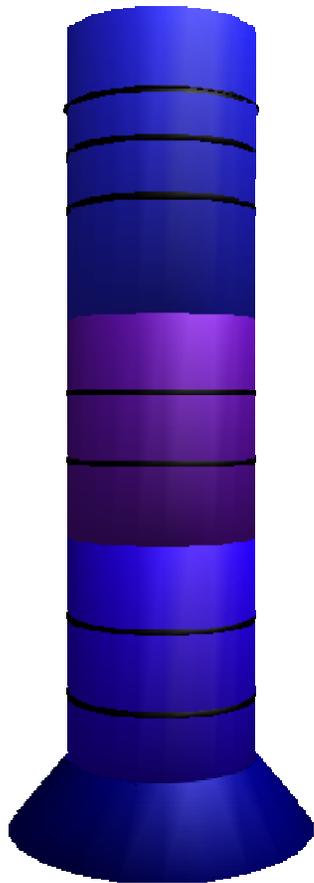
diffuse scattering



x-rays, neutrons

Next Generation Lorentz Microscopy

world-class imaging of magnetic/electric structure with sub-nm resolution



Schottky FEG

Monochromator

Condenser

C_s corrector

LIS Objective

Specimen + Stage,
10 mm gap

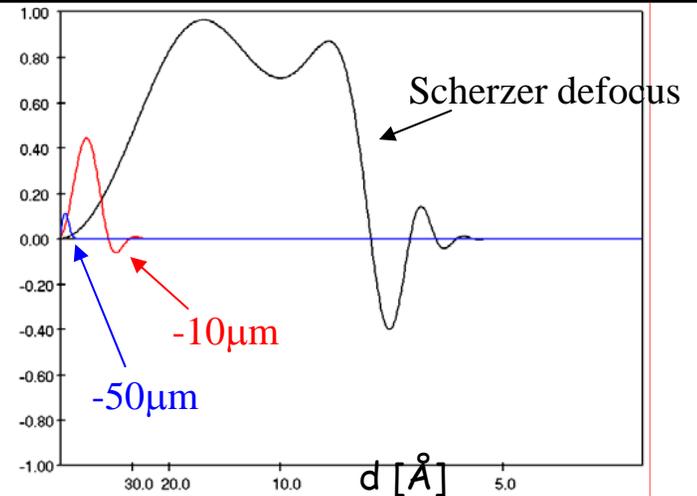
LIS Objective

C_s and C_c corrector

Energy filter

Projectors

Fast CCD-system

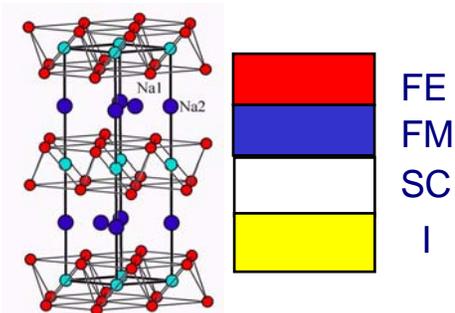


implementation plan

- JEOL column
 - spherical aberration correction: commercial
 - novel Lorentz image reconstruction
 - chromatic aberration correction: TEAM spin-off
- system within reach

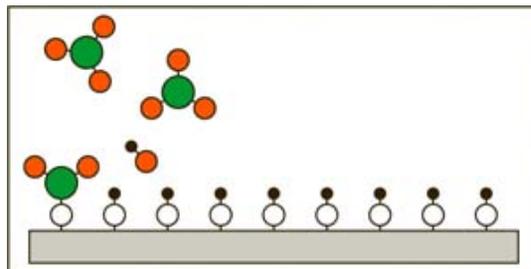
Amanda Petford-Long, Bernd Kabius, Nestor Zaluzec, Dean Miller

Atomic Layer Deposition: Digital Synthesis/Coating

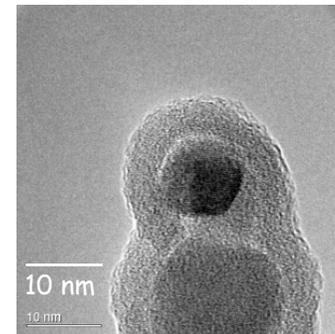


create mixed oxides

layer by layer deposition

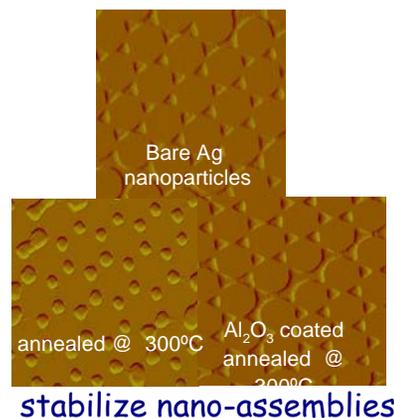
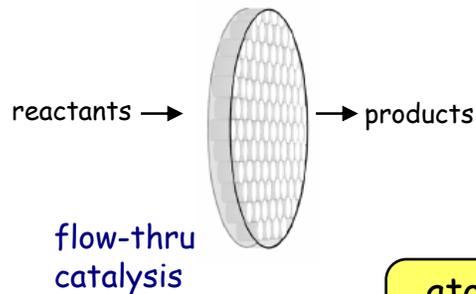
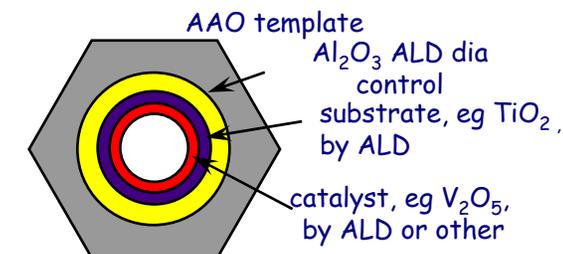
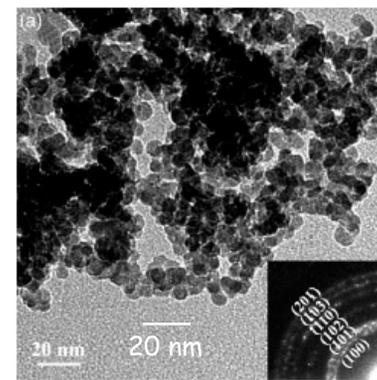


4 nm TiO₂ on ZrO₂



conformal coating of complex objects

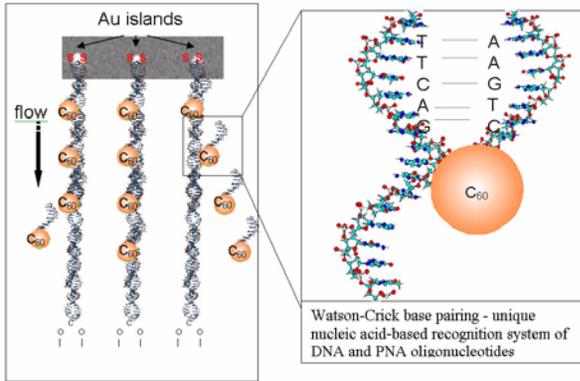
ZnO on silica aerogel



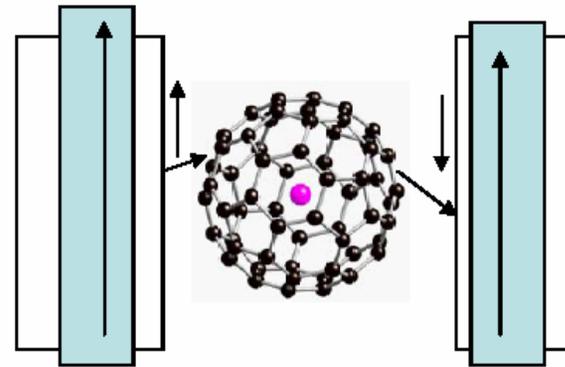
atomic level control of synthesis and sequential coating of AAO, aerogel, and mesoporous materials.

Electron Spin Quantum Computer

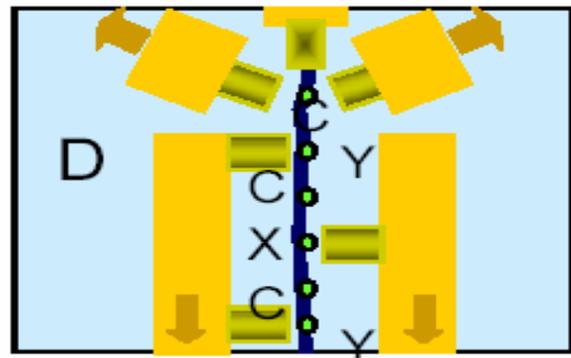
DNA Template for N-C60



Radio Frequency Single Electron Spin Transistor



Dip Pen Nano-lithographic Gates & Junction



interdisciplinary nanoscience
confinement, complexity, bio-interfaces, directed self-assembly

Science Driving Facilities

Electrons

- Ultracorrector electron optics (*Kabius*)
- Lorentz imaging of magnetic/ferroelectric domain reversal (*Petford-Long, Kabius, Zaluzec*)
- in situ electrocatalysis (*Markovic, Zaluzec*)

Neutrons

- SERGIS spin echo resolved grazing incidence spectroscopy polymer and bio-membranes (*Felcher, te Veltuis*)
- diffuse scattering of short range and complex disorder (*Rosenkranz, Osborn, Kirk*)

Science Driving Facilities

X-Rays

- high resolution powder diffractometer (APS)
synthesis-characterization (*Mitchell*)
- in situ MOCVD (APS) \Rightarrow GaN (*Streiffer, Stephenson*)
- in situ oxidation (APS) (*Eastman*)
- in situ electrocatalysis (*Markovic, You*)
- nanoprobe \Rightarrow 30 nm diffraction/spectroscopy (*Stephenson, CNM*)
- in situ MBE (*Auciello, Schlom, Streiffer, et al*)

Extensive experimental use at all facilities

Education and community building

- Neutron and X-Ray Scattering School (*Osborn*)
- Future: Electron Scattering Science School (*Miller, Zaluzec*)

Strategic Materials Partnerships

with Universities

UC: joint position search, CNR

UIC: J. C. Campuzano (Phys)

NU: Peter Stair (Chem), catalysis

Amanda Petford-Long, mat sci

NIU: Zhili Xiao (Phys), nanosynthesis

Notre Dame: ITS (B. Janko)

IIT/Russia, Taiwan: graduate students

within ANL

CHM: L. Curtiss, P. Zapol, X.-M. Lin *joint appts*

BIO: magnetic viruses, bio-scaffolds

CNM: B. Stephenson, *Nanoprobe Leader*

S. Bader, *Scientific Director*

S. Streiffer, *Systems Coordinator*

A. Hoffmann, P. Zapol, J. Carlisle,

D. Gruen, O. Auciello, *Theme Leaders*

CMT: D. Myers, *BES Hydrogen Proposal*

with User Facilities

IPNS J. Jorgensen, S. te Velthuis, R. Osborn, *Inst Spec*

G. Felcher, *SERGIS*

S. Rosenkranz, R. Osborn, *Diffuse Scattering*

APS B. Stephenson, *Nanoprobe*

J. Mitchell, *Powder Diffractometer*

J. Eastman, P. Fuoss, H. You, *science programs*

EMC D. Miller, *Director*

B. Kabius, *TEAM electron optics coordinator*

+ A. Petford-Long *electron scattering science*

with BES

M. Norman, *BESAC Theory/Modeling Report*

G. Crabtree, *Energy Security, Hydrogen, Solar*

I. Aronson, S. Bader, O. Auciello, J. Carlisle, J. Mitchell, *CSP Project Leaders*

R. Osborn, *Neutron and X-Ray Summer School*

J. Mitchell, S. Rosenkranz, R. Osborn, Gian Felcher, *Instruments for SNS, APS*

J. Mitchell, P. Canfield, J. Sarrao, D. Gibbs, D. Mandrus, *Materials Synthesis Network*

BES Funding

FY05 initial decrease: 7.1%

FY05 increase to date: 7.8% ~ \$130K

Neutron scattering

Emerging materials

Synchrotron studies

Interfacial materials (Petford-Long)

Pending

Synchrotron studies (Markovic)

Electrocatalysis for hydrogen economy (You)

Theory (Matveev)

Quantum computing (Fradin)

Bio-granular dynamics (Aronson)

models for growing programs - we need more of this!

Strategic Hires

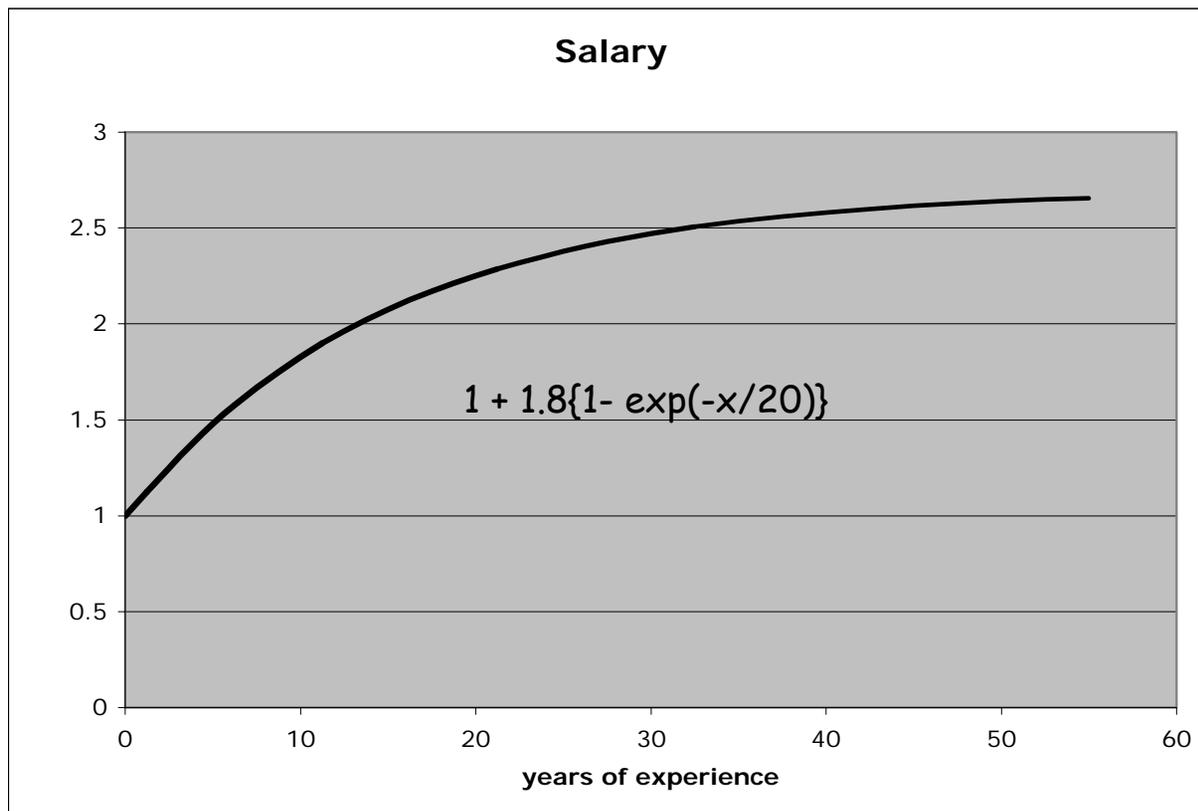
- *Amanda Petford-Long*
 - visited in April, move permanently August
 - partial BES support for salary, program
 - invited white paper for Lorentz imaging purchase
 - invited \$1M proposal after arrival
- *Nenad Markovic*
 - visit June 20-24, tentative move August
 - BES support for program
 - invited \$1M proposal after arrival
- *Uzi Landman*
 - joint UC
 - negotiation for program resources

Future Path

- propose world-class science to BES
 - highlights \Rightarrow white papers \Rightarrow proposals \Rightarrow highlights
 - solar energy conversion
 - *electricity- quantum dots, dye sensitized, redox couple*
 - *chemical fuel- biomolecular catalysis*
 - *thermal concentrators*
 - LDRD as stepping stone
- career advancement: how to succeed in MSD
 - propose and lead world-class science: new FWP
 - propose and join world-class science: FWP team

Raises and Bonuses

divisional salary profile



experience factor

$x \sim 4$ 0.8

$x=12$ 0.55

$x=25$ 0.3

raise pool = 2.5%

early > 2.5%

late < 2.5%

bonus pool = 1.9%

Lab policy

D evaluations limited by quota
bonuses to D performers + 10% of C's

New Faces and Appreciation

new since September 2004

- 13 postdocs
- 3 visiting scientists
- 8 summer students
- 2 summer faculty

service awards

5 years: 1	25 years: 2
10 years: 3	30 years: 4
20 years: 1	35 years: 1
40 years: 1	

News Updates

- Research Highlights CD

<http://www.msd.anl.gov/highlights/index.html>

Ulrich, Paul, Urs, Dave Lehman. Marlene, Suzanne

- New microscopy building - SAMM \$2.5M BES/\$2M ANL

- Strategic Initiative: Energy Environment, Prosperity

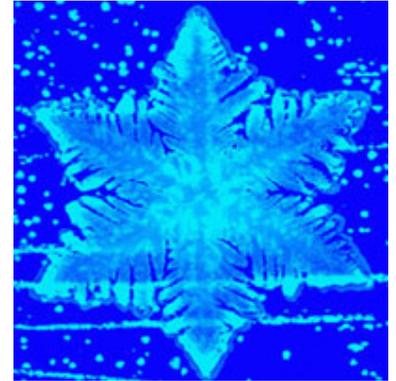
- BES Solar Energy Initiative - report summer 05, proposal call June 06

- Interim conversations, by June 30

- Institute of Theoretical Science Notre Dame/Argonne

Room Temperature Superconductivity Notre Dame June 10-11

- CNM: \$4M operating funds in FY06



Questions and Reception

Congratulations

Hoydoo You, Nenad Markovic, Goran Karapetrov,
Zoltan Nagy, Peter Zapol, Debbie Myers (CMT),
Yuri Tolmachev (Chemistry, Kent State U)
Woods Halley (Physics, U Minnesota)