UEC Dinner meeting 09/16/2014

Location: SNS CLO, Room C-156

Meeting convened 18:40

UEC Members Attending: Vivek Prabhu, Nazanin Bassiri-Gharb, Zheng Gai, Martyn McLachlan, Megan Robertson, Ray Unocic, Rafael Verduzco, Tony Hmelo
Non-Members Attending: Hans Christen, Bobby Sumpter, Tony Haynes, Viviane Schwartz

Hans presented a briefing on the state of the CNMS (slides attached) and we discussed some of the statistics about funding and users. There was also some discussion about how to diversify the user base to include a higher percentage of users from more distant parts of the country. We discussed ways to increase participation by industrial users. Suggestions were: holding an industry workshop seeded by participation of current industry users; the workshop could include lab demos where participants bring their own samples (like a mini-Rapid Access project, with take-home results, and include participation by DOD and/or SBA researchers and/or Program Managers for their network of industry contacts as part of the workshop.

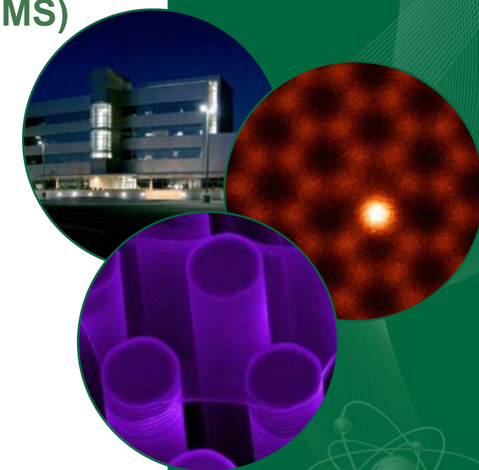
Vivek presented the briefing for the Town Hall meeting during 9/17/14 CNMS user meeting. There were a few minor changes suggested. Final slides will be posted in the User Group area of CNMS website.

Nominations for UEC election:
* A pending nomination of Molly Kennedy for Vice Chair was seconded by Nazanin Bassiri-Gharb
* Two new self-nominations for At-Large positions were submitted by Rafael Verduzco and Megan Robertson; both were seconded by Martyn McLachlan
*All nominations at this time were added to the Town Hall slides

Student Poster Awards:
*Milan summarized the student poster award scores and presented the top candidates.
*UEC approved the top candidates, without modification, and the results were included into the Town Hall Slides.

Meeting adjourned 20:45

Center for Nanophase Materials Sciences (CNMS)



"State of the CNMS"
Presentation at the UEC Dinner Meeting, Sept. 16, 2014

Hans Christen
CNMS Director

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News and activities

- No feedback yet from triennial review
- Strategic plan revised, presented at DOE-HQ, and approved as-is
- Formation of Soft Matter Council, hiring activities
  - Offer accepted for junior staff position
  - Ongoing search for a senior staff position
- Institute for Functional Imaging of Materials (IFIM). Director: Sergei Kalinin

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Budget outlook (from July BESAC meeting)

President's request: SUFD +3.6%, CNMS +6.4%

FY 2015 BES Appropriations: HEWD vs. SEWD

HEWD Mark

	FY 2014 Approp.	FY 2015 Request	FY 2015 House	FY 15 House vs. FY 14 Approp.		FY 15 House vs. FY 15 Request	
BES Total	1,711,929	1,806,5[illegible]	1,702,000	-9,929	-0.6%	-104,500	-5.8%
MSE & CSGB	678,765	70[illegible]	662,662	-16,103	-2.4%	-40,194	-5.7%
SUFD	931,164	964,944	911,338	-19,826	-2.1%	-53,606	-5.6%
Construction	102,000	138,700	128,000	+26,000	+25.5%	-10,700	-7.7%

- BES research is held approximately flat with FY 2014, including EFRCs and the Batteries Hub.
- No funding for the Fuels from Sunlight Hub.
- $8M for computational materials sciences.
- The LCLS-II construction project is funded at $128M, $10.7M below the FY 2015 request.
- Major items of equipment and the neutron scattering facilities are funded at the FY 2015 request level.
- NSLS-II operations funded at $105M, $10 below the request.
- Due to the language included the House mark, reductions must be taken from the light sources and nanoscale science research centers, resulting in ~10% reduction for these facilities compared to the FY 2015 request.
- $10M for the DOE EPSCoR program, $1.5 M above the request.

= 4.2% cut wrt. 2014

SEWD Subcommittee Mark

	FY 2014 Approp.	FY 2015 Request	FY 2015 Senate	FY 15 Senate vs. FY 14 Approp.		FY 15 Senate vs. FY 15 Request	
BES Total	1,711,929	1,806,500	1,806,500	+94,571	+5.5%	—	—
MSE & CSGB	678,765	702,856	703,161	+24,396	+3.6%	+305	+0.04%
SUFD	931,164	964,944	964,639	+33,475	+3.6%	-305	-0.03%
Construction	102,000	138,700	138,700	+36,700	+36.0%	—	—

- The Senate mark provides funding for all of the activities requested in FY 2015.
- $18M for computational materials sciences, $6.2M below the request.
- The Senate mark fully funds ramp-up of NSLS-II operations.
- All construction and MIE projects are funded at the requested levels.
- $15M for the DOE EPSCoR program, $6.5 M above the request.

= 6.4% increase wrt. 2014

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The CNMS: a unique combination of research effort and user facility

- One of 5 Nanoscale Science Research Centers created by the DOE as contribution to the U.S. Government National Nanotechnology Initiative (NNI)
- Started operations in 2006; merged with ShaRE (Shared Research Equipment User program) in 2014.
- Influx of visitors brings ideas, interactions, exciting and stimulating environment
- Researchers balance work on in-house research with work on user projects
  - 50% of staff time committed to working with users
    50% of staff time committed to in-house science
  - 80% of instrument time dedicated to users
    20% of instrument time for in-house science

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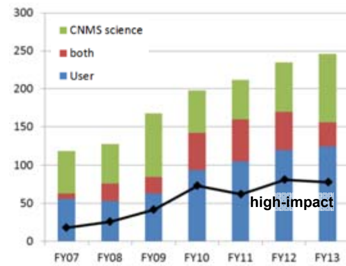
  - 80% of instrument time dedicated to users
    20% of instrument time for in-house science
- Performance Metrics:
  - Number of users: Expectation for FY2015: 500
  - Number of publications



"High-Impact" journals (20):
Science, PNAS, PRL, JACS, ACS Nano
Nature, N. Chem., N. Materials, N. Nanotech., N. Photonics, N. Phys., N. Comm.
Adv. Mater., Adv. Funct. Mater.
Small
NanoLetters
Nanoscale
Angew. Chem. Int. Ed.
Chem. Mater.
Appl. Phys. Lett.

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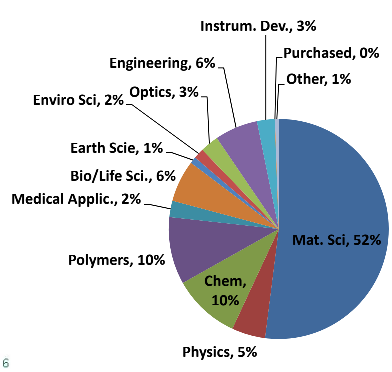
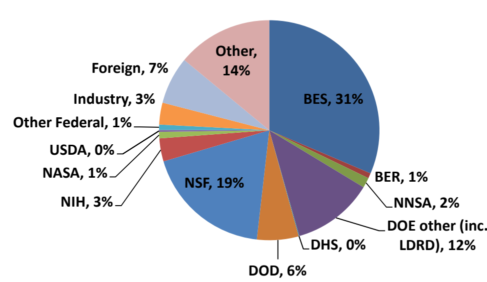
Who are the CNMS users?

What users come to the CNMS for:

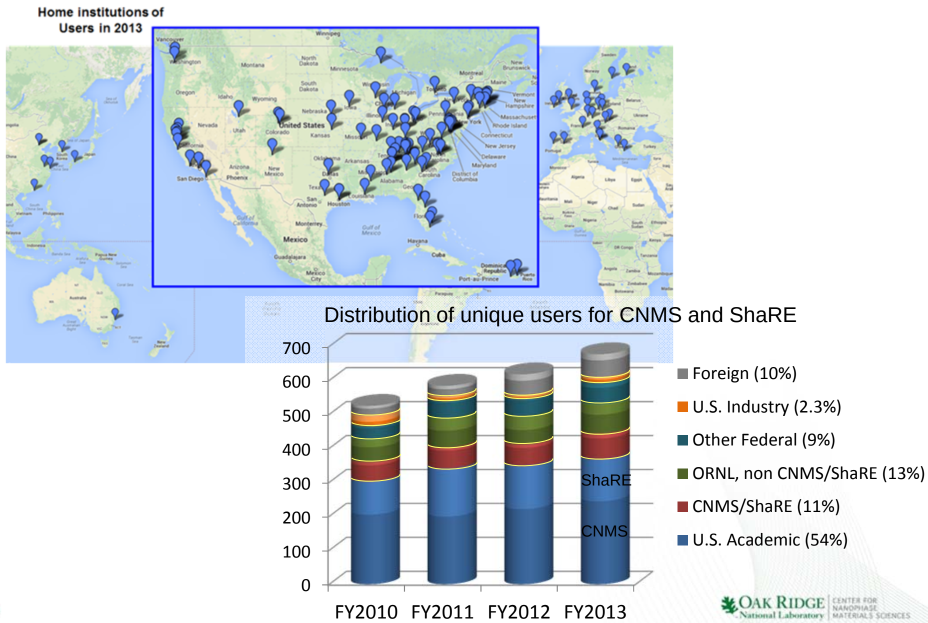
- 10% theory
- 40% (synthesis or fabrication) *and* characterization
- 50% characterization

What the users want from us
(Word cloud of all text in the "work to be performed at the CNMS or ShaRE" text boxes in the proposals)

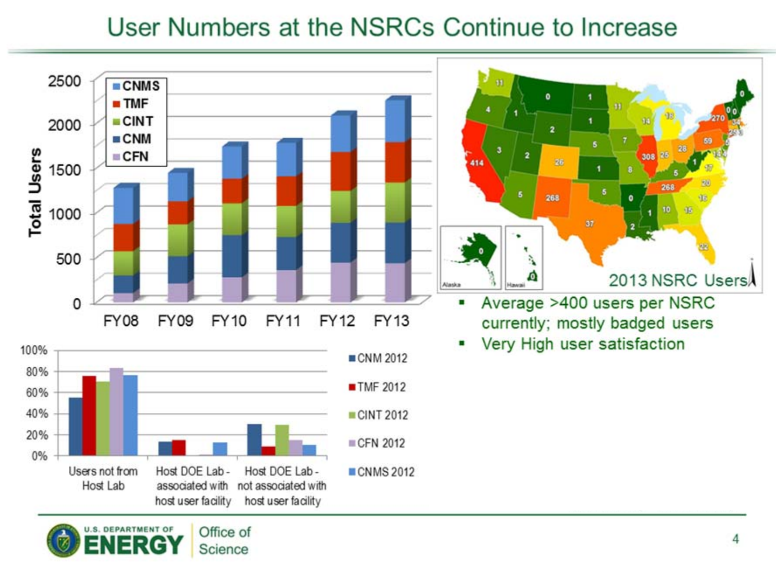




The CNMS has a geographically broad user base



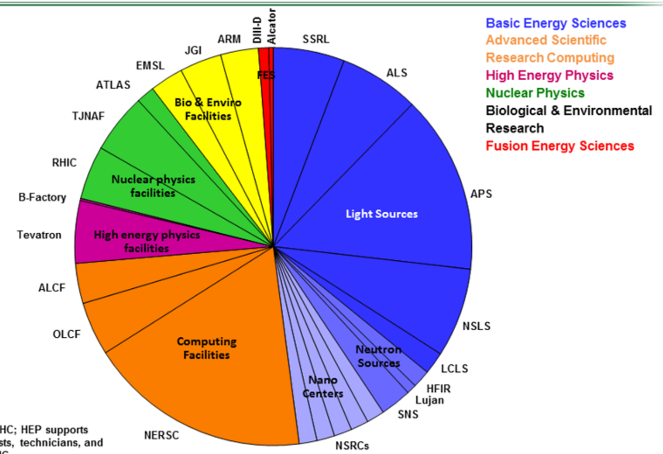
From the spring BESAC meeting (Harriet Kung)



From the spring BESAC meeting (Pat Dehmer)

Distribution of Users at the ~30 SC Facilities 2013

Nearly ¾ of users do their work at ASCR or BES facilities



Does not include LHC; HEP supports about 1,700 scientists, technicians, and engineers at the LHC.

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Outreach for non-local and industry users

- **General Outreach**
  - The most effective modes of outreach are conference presentations and publications by staff and users who acknowledge CNMS
  - User meeting as a open forum to discuss opportunities
- **Targeting Industry**
  - Help prospective industry users understand how to frame the basic, publicly reportable scientific principles that underpin their R&D challenges in order to strengthen their user proposals
  - Success rate is >40% for user proposals from industry. Need to encourage re-submissions.
  - One effective strategy is to start small with Rapid Access to get a new industry user “in the door”
  - Work with industry partners to explore alternative cooperative mechanisms such as CRADAs or WFO
  - Engage in industry outreach activities led by applied research programs at ORNL, where industry contacts are very well established

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The CNMS "group and theme" structure

- The groups are responsible for *capabilities* and for *interaction with users*:
  - Imaging and Nanoscale Characterization / Scanning probes
  - Microscopy / STEM, APT
  - Nanomaterials Synthesis and Functional Assembly
    - Functional Hybrid Nanostructures / Optoelectronics
    - Macromolecular Nanomaterials / Polymers
    - Chemical Functionality / Catalysis
  - Nanofabrication
  - Nanomaterials Theory Institute
- The in-house research has the goal of *understanding and controlling the complexity of electronic, ionic, and molecular behavior at the nanoscale* to enable the design of new functional nanomaterials - 3 "themes""
  - Electronic and ionic functionality at the nanoscale
  - Functional polymer and hybrid architectures
  - Collective phenomena in nanophases
- Integration with computation, neutrons, and imaging is key to the success of the CNMS

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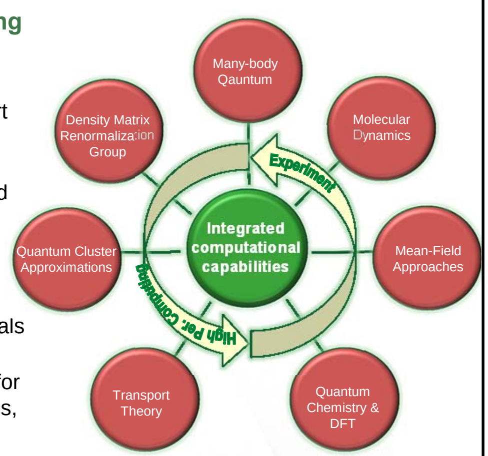
The Nanomaterials Theory Institute integrates within the CNMS and links to other ORNL efforts

Developing a fundamental understanding of control over physical and chemical properties to build responsive matter

- Understanding and rational tuning of transport (electron, spin, ion, molecule), reactivity and electronic structure
- Developing methodologies for theoretical and computational nanoscience to establish new capabilities and to enhance links with experiment
- Building the scientific foundation to study and design functional correlated electronic materials (such as superconductors)
- Advancing soft matter theory and simulation for understanding morphology, stability, dynamics, and properties of topologically complex multiblock and charged copolymers, brushes, composites and blends



The NTI builds a tight connection to computational sciences

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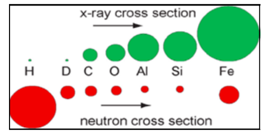
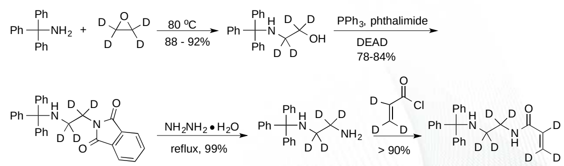
Linking synthetic capabilities to neutron sciences: Precise synthesis and deuteration

- **Selective deuteration: ability to replace H with D at selected positions to optimize contrast in neutron scattering experiments, and to elucidate the structure and dynamics of soft matter**

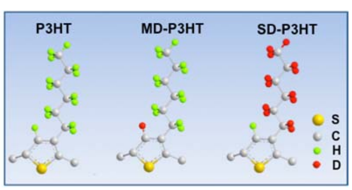


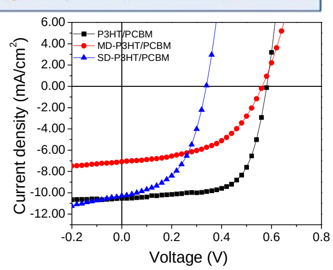
- **Atom-efficient synthesis: The synthesis of partially or fully deuterated analogs of a variety of molecules (monomers, surfactants, polymers, dendrimers, etc.) in a atom-efficient and cost-effective manner often requires the development of novel synthetic strategies that are different from those used to make non-deuterated molecules**



13 Yang et al., "Synthesis of N^1-tritylethane-*1,1,2,2-d$_4$*-1,2-diamine: a novel mono-protected C-deuterated ethylenediamine synthon," *J. Labelled Compd. Radiopharm.* **55**, 463 (2012).

Isotopic effects of deuteration on the optoelectronic properties of conducting polymers





Top: Chemical structure of P3HT, and its main-chain (MD-P3HT) and side-chain (SD-P3HT) deuterated isotopes.
Bottom: Distinctly different J-V characteristics of the three P3HT isotopes in $PC_{60}BM$ blend photovoltaics.

Ming Shao et al., *Nature Commun.* **5** 3180 (2014)

Scientific Achievement

We show that selective substitutions of deuterium (D) on the backbone or side-chains of conducting polymer poly(3-hexylthiophene)s (P3HT) significantly change their optoelectronic response in P3HT/PCBM ([6,6]-phenyl-C61-butyric acid methyl ester) photovoltaics.

Significance and Impact

Our work shows that isotopic substitution, once thought to be a benign modification, provides a new means to tune the optoelectronic properties of conducting polymers used for solar cells by affecting their intra- and inter-polymer chain interactions.

Research Details

- Developed a series of P3HT isotopes by selectively substituting deuterium on the backbone (MD-P3HT) or alkyl group (SD-P3HT).
- Integrated approaches including neutron/x-ray scattering, TEM and theoretical modeling were used to understand the origins of the large effects of D on the optoelectronic and structural properties.

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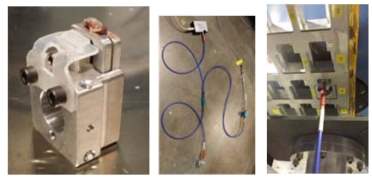
Strong CNMS-neutron interactions

18% of CNMS users are also SNS or HFIR users

- **CNMS staff are collaborating with the SNS to develop in-situ environments for neutron scattering**

Example: cell for in-situ PL on EQ-SANS



- **Simplified access to SNS/HFIR for CNMS users – and vice versa**
  - **"Proposal appendix" – essentially a joint submission of a proposal to both institutions**
  - **Recognizing science reviews from the sister institutions (identical reviewer questions / scales)**

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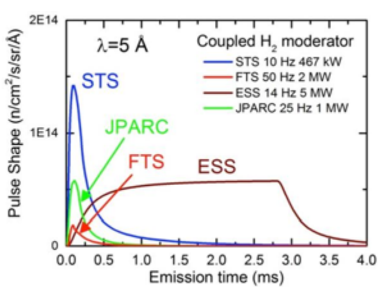
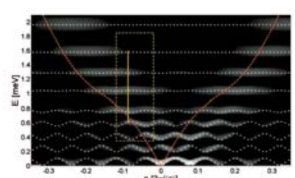
The Second Target Station will meet future science objectives in nanoscience

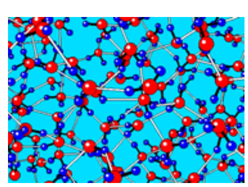
- **Cold neutrons: long wavelengths for the study of larger scale phenomena and slower dynamics**
- **High brightness beam and beam focusing to work with smaller samples**



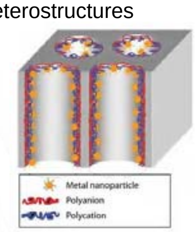
Superior peak brightness for cold neutrons



Artificial crystals and heterostructures



Reactions, catalysis, and kinetics



Hierarchical materials

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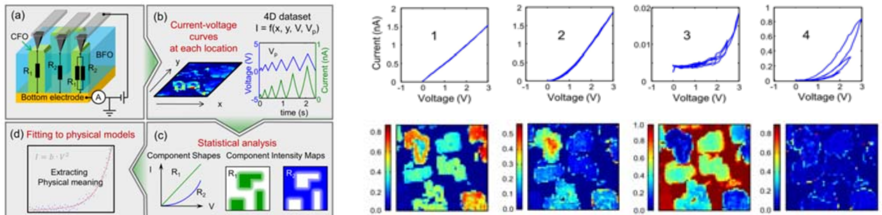
The ORNL Institute for Functional Imaging of Materials (IFIM)

- Imaging has evolved from "observing where atoms sit" to locally (actively) interrogating the behavior of a material; truly multidisciplinary
- Data sets are multi-dimensional and can't simply be plotted



E. Strelcov *et al.*, *ACS Nano* **(2014)**

- Specific imaging/data challenges:
  - Extracting information
  - Distinguishing between noise and data
  - Merging data streams (e.g. STEM and APT)
- IFIM integrates imaging priorities across ORNL and builds the connection between imaging and computational sciences
- IFIM assures that DOE gets the highest benefit from current and future microscopy investments

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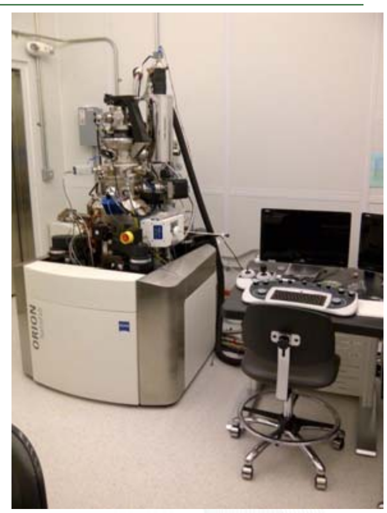
Zeiss Orion NanoFab: the first He$^+$ microscope dedicated to nanofabrication

- Highest resolution ion-milling tool available
- Two ion choices: He+ and Ne+
- Built-in patterning capability
  - Resist patterning
  - Ion milling
  - Located in CNMS cleanroom
- High-resolution scanning ion microscope
- Currently installing: beam-induced direct write of metals
- Future opportunity: Combination with mass spectrometry



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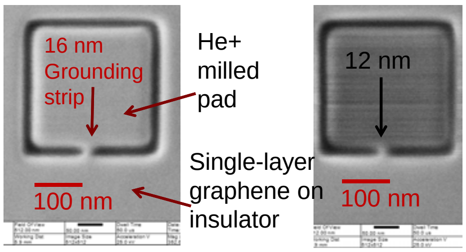
He$^+$ microscope - examples:

Transport effects in single-layer graphene (CNMS staff, unpublished)

- Constriction of graphene strip reduces electron flow in situ (charging)

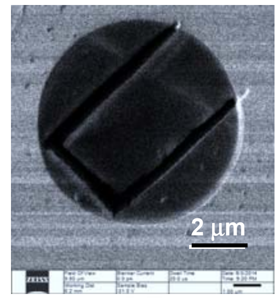


- Demonstration that 16 nm wide features in *supported* graphene are possible (damage margin < 8 nm)

Ne$^+$ milling of a single-layer graphene cantilever (CNMS user)

VANDERBILT

Courtesy:
Kirill Bolotin

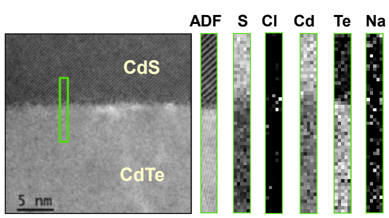


- Free-standing, 5 µm cantilever
- Ne$^+$ milled (no resist, no Ga)

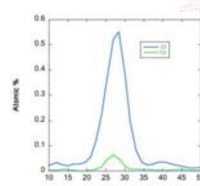
Atom-Probe Tomography

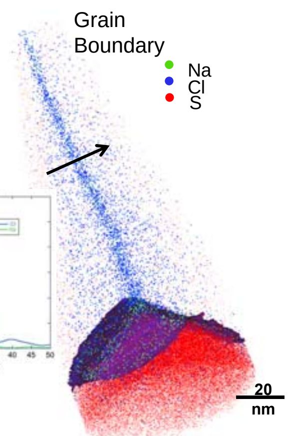
Laser-LEAP (local electrode atom probe): complete 3D reconstruction of atomic positions and atomic masses

- No longer limited to metallic samples
- Sensitive to *any* element (detecting light elements within a disordered matrix of heavier elements)



EELS elemental maps of CdTe/CdS interface
No Na detected at interface

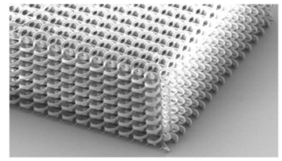




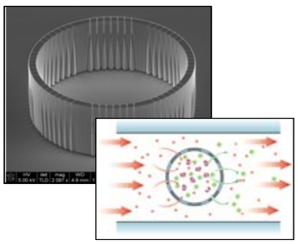
- Strategic-hire investment
- Future upgrades for improved detection efficiency

Future priority: fabrication of 3D structures

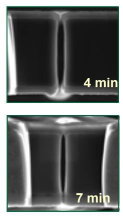
- Proposed tool: Nanoscribe Photonic Professional GT



- Complex structures can be fabricated by 3D direct write laser lithography in combination with ALD and direct-write capabilities (EBID, He⁺).

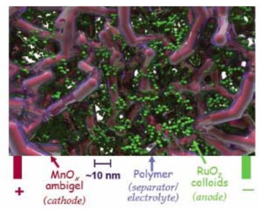


Confined chemistry experiments: currently limited to 2D



ALD used to control pore size

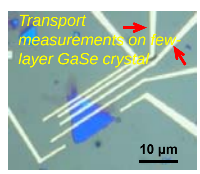
3D structures with controlled feature size and connectivity

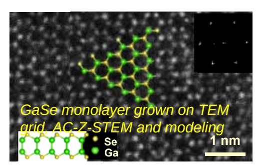


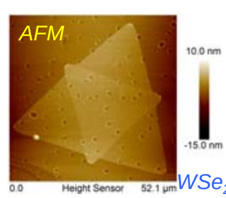
Work by others proposes 3D battery structures (Long et al., 2004)

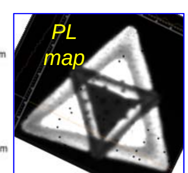
Future priority: Ultrafast phenomena

- 2D materials (graphene, metal chalcogenides) are excellent platforms to explore interfacial interactions
- The fundamental optoelectronic processes at interfaces are relevant to photovoltaics, lighting, sensors…
- CNMS has built the expertise to synthesize and characterize 2D materials



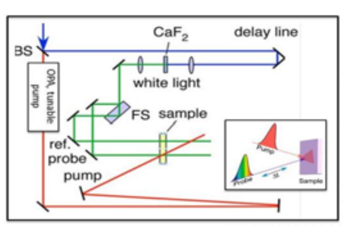


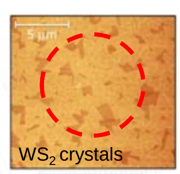




WSe_2

- Current capabilities allow us to probe time-dependent phenomena using 40fs pulses, 10 µm (w.l.) to 1 µm (OPA) spot size

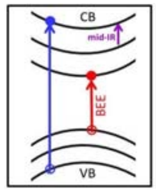


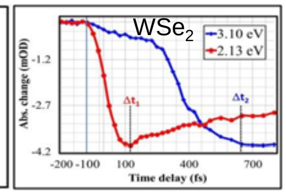


Future priority: Ultrafast phenomena (cont.)

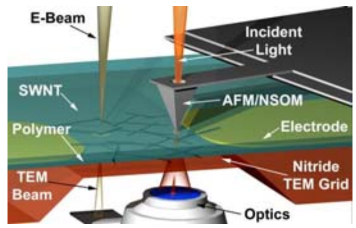
Faster and smaller:

- **Determining time-scales for band-edge exciton formation requires sub-10fs laser pulse widths**

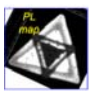




- **Addressing processes at edges in 2D materials, and at individual 0D and 1D nanostructure interfaces requires the integration of ultrafast spectroscopy into an NSOM platform**



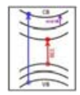
Ultrafast measurements probe the quantities that can be calculated, and therefore form a critical link to theory/modeling/simulation.



Synthesis
Imaging
Properties

⟷ Ultrafast ⟷

Theory
Modeling
Simulation



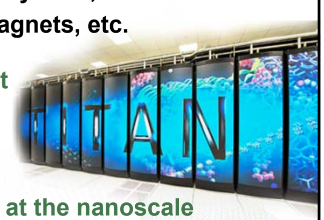
Materials by Design

There are no known fundamental barriers that prevent us from reaching the goals of

- **Reduced cost and increased efficiency of solar cells**
- **Increased energy and power densities in batteries**
- **Higher strength in lightweight (nano)composite materials**
- **Efficient direct catalytic conversion of sunlight to fuels**
- **…**

We do not have the time or resources to explore all the options experimentally:

- **Many degrees of freedom in composition, structure, and dynamics**
- **Billions of chemical combinations for catalysts, polymers, etc.**
- **Increased complexity in new superconductors, magnets, etc.**

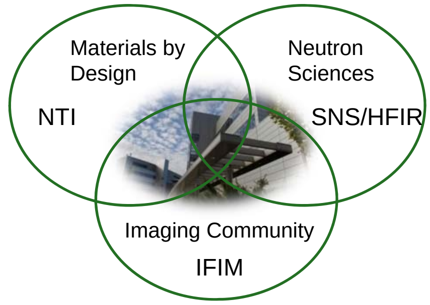


- **Computational capabilities have advanced to a point where Materials-by-Design strategies can (and will) be explored**
- **Imaging approaches provide the key information**
- **The first true Materials-by-Design successes will be at the nanoscale**

The Center for Nanophase Materials Sciences

Providing access to state-of-the-art nanoscience research capabilities by building on CNMS foundational strengths and the ORNL environment

Understanding and controlling the complexity of electronic, ionic, and molecular behavior at the nanoscale will enable the design of new functional nanomaterials.



Foundational strengths in synthesis and fabrication:
- Soft matter synthesis/deuteration
- 2D materials/ultrafast dynamics
- 3D structures/confinement
- Controlled nanostructures/layers

Foundational strengths in theory, modeling, simulation:
- Transport, reactivity, electronic structure
- Correlated electron materials
- Soft matter theory/simulation

Foundational strengths in imaging:
- Scanning probe microscopies
- Scanning transmission electron microscopy
- Atom-probe tomography
- He+ microscopy

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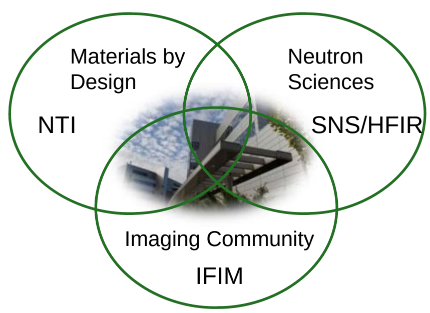
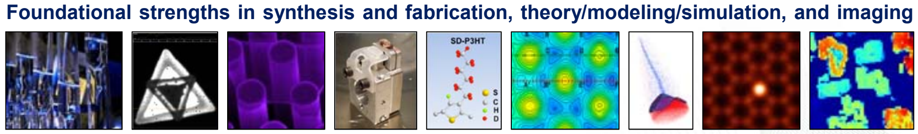


Foundational strengths in synthesis and fabrication, theory/modeling/simulation, and imaging



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