2017 CINT Annual Meeting

SAND2017-10487C

September 25-27, 2017

La Fonda Hotel, Santa Fe, NM

http://cint.lanl.gov

CINT Core Facility

CINT Gateway Facility

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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Introductions and CINT Updates

- Welcome
- Joint NSRC Workshop on Soft Matter
- CINT's Vision
  - New Staff
  - Current Openings
  - New and planned capabilities
- Brief user stories

CINT's Vision

Provide access to *scientific expertise* and *advanced capabilities* to synthesize, fabricate, characterize, understand and integrate nanostructured materials into the microscopic and macroscopic worlds

Inspire technological innovation with enduring beneficial impact in energy, environment, human health and security

For more information also see CINT 2022 Strategic Plan on our website

Familiar Faces, New Roles

Jim Werner
Deputy Group Leader
Gateway

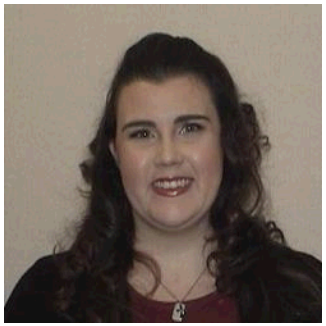
Brian Swartzentruber
Manager
Core

Mike Lilly
NEM Thrust Leader
Core

Jinkyoung Yoo
Thrust co-Leader
Gateway

New Personnel

Andreas Roelofs
CINT-Director
Gateway



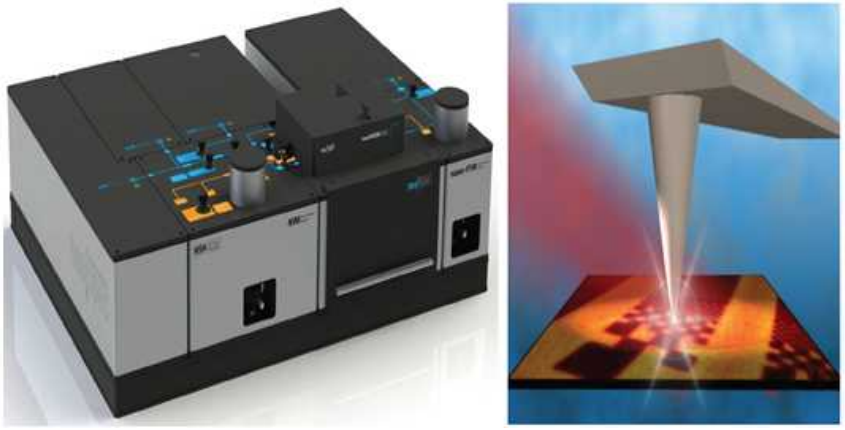
Jacinda Matthews
Administrative Assistant
Core

Sarah Eccleston
Administrative Assistant
Core

3 scientists openings
Hiring and outreach coordinator

New Capabilities in Near Field Microscopy and Magneto-Spectroscopies

NeaSPEC scanning near-field optical microscope



Flexible coupling to light sources.

- Far-infrared to visible.
- fs time resolution pump-probe

Dynamics in broad materials systems:

- Strongly correlated materials
- Plasmonics and wave properties in 2D
- QDs, nanowires, and carbon nanotubes
- Metamaterial resonances

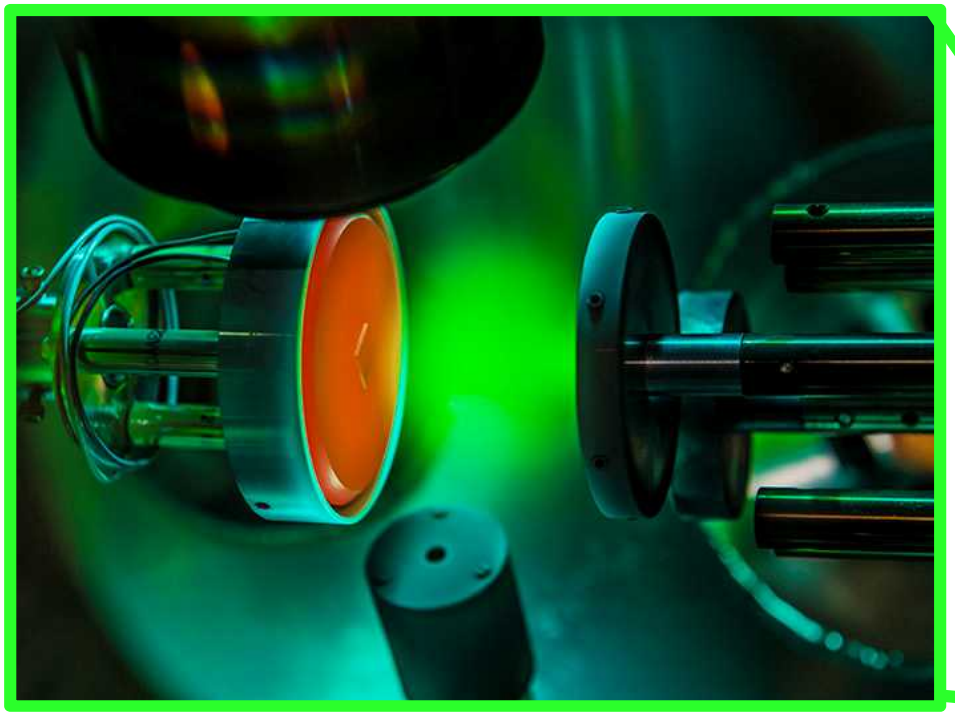
Janis 9 T superconducting magnet and microscopy cryostat

Nanostructure magneto-PL & Raman.
Time-resolved and correlation spect.

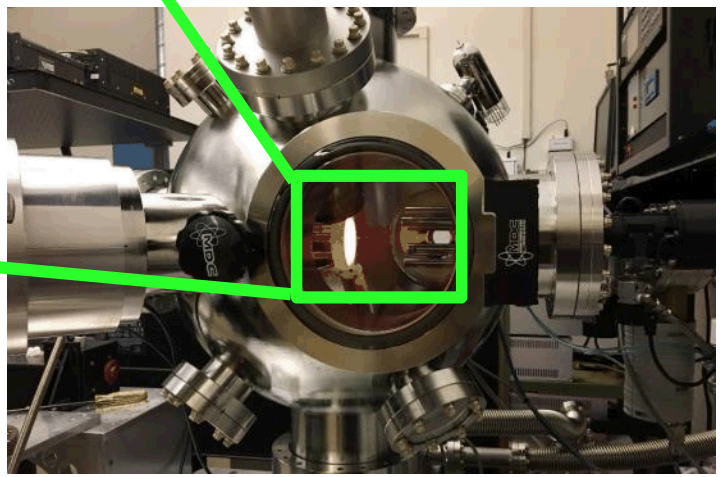
Single Nanostructure studies:

- 2D materials (graphene TMDCs)
- Semiconducting nanostructures
- Complex metal oxide films

New Capabilities in Pulsed Laser Deposition



Dual laser PLD system enables deposition of thin films and nanoparticles



Growth of **Oxide Superlatices** and **Vertical Nanocomposites,** including **Actinides**

New TEM Capability!

Titan ETEM G2

- Image corrected
- Monochromated
- Environmental
- Lorentz imaging (magnetic samples)
- Gatan K2-IS high-speed / low dose camera
- Piezostage for fine samples control
- In-situ holder compatible

On-line for users Spring 2018

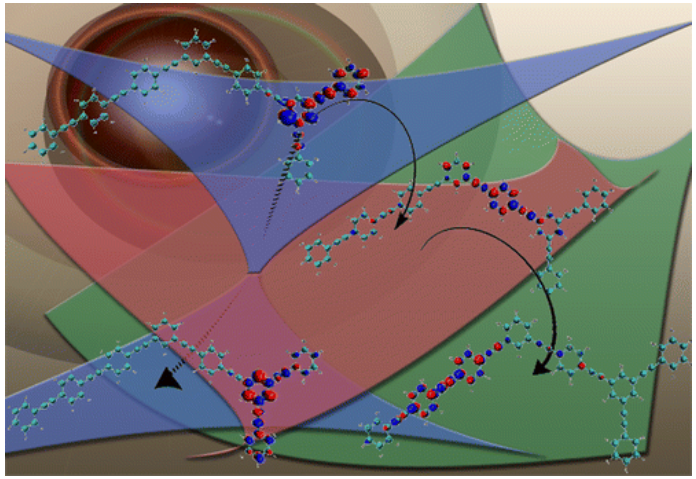
Modeling capability

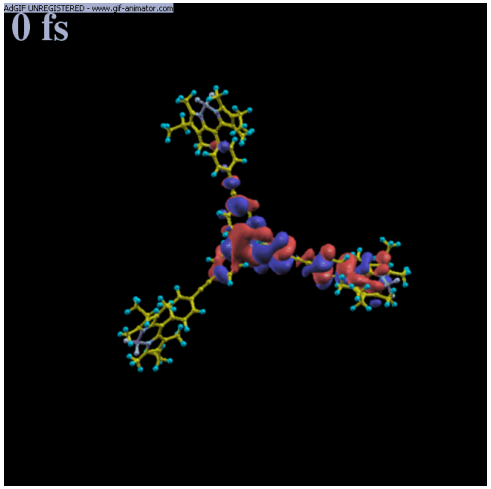
- **Non-adiabatic EXcited state Molecular Dynamics (NEXMD) package is a unique modeling tool for photophysics and photochemistry in the presence of environment (QM/MM)**

- Started in 2009 as international user project
- Over 100 publications (Acc Chem Res (2014), Chem Rev (2015), Chem Rev (2018)
- Being routinely used by ~15 user projects at a time

Adrian Roitberg (U Florida)

Sebastian Fernandez-Alberti (Buenos Aires)





- **Major Milestone:**

stated for public release in 2017 with help of LANL Feynman center

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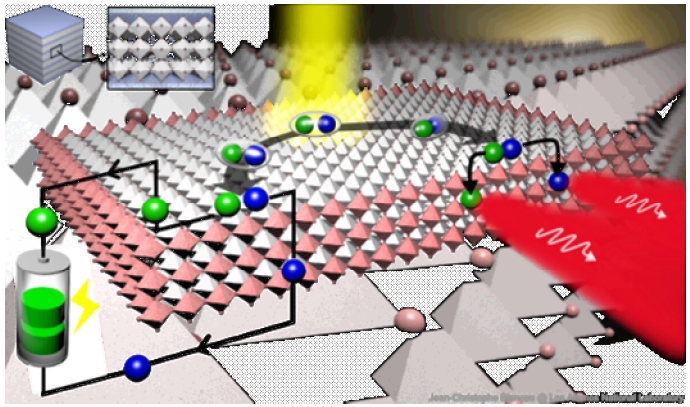
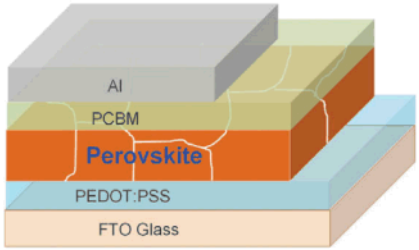
Experiment-Theory collaboration

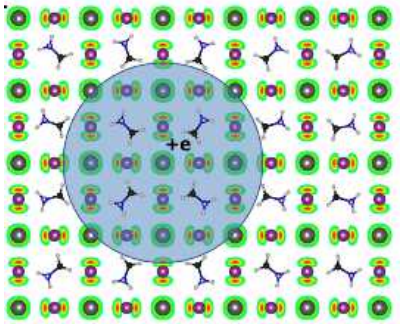
- **Hybrid perovskites for optoelectronic applications**

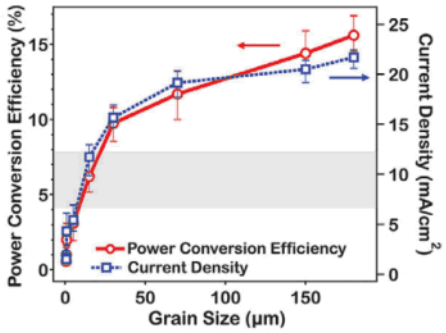
Aditya Mohite (LANL)

- Started in 2014 as internal LANL user project with A. Mohite
- Over 20 publications (Science (2015), Nature (2016), Science (2017)
- About 10 new user projects from Spring 2017 cycle
- 5 DOE highlights since 2015









- **Became among top 3 perovskite programs in the country**

Our future modeling capability

• Machine Learning and Informatics for nano-materials

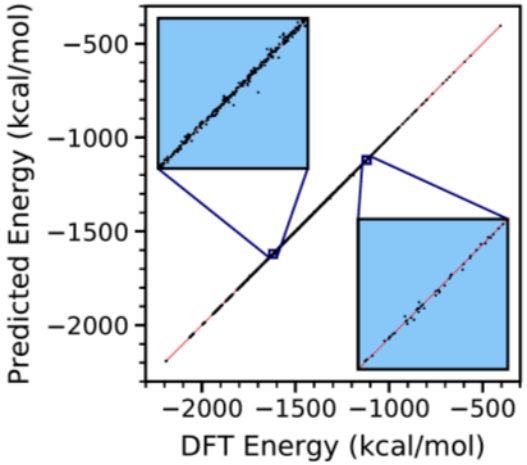
• Started in 2017 as internal CINT research

• Aiming to scalable new generation of atomistic sinulation tools (exascale computation and co-design)

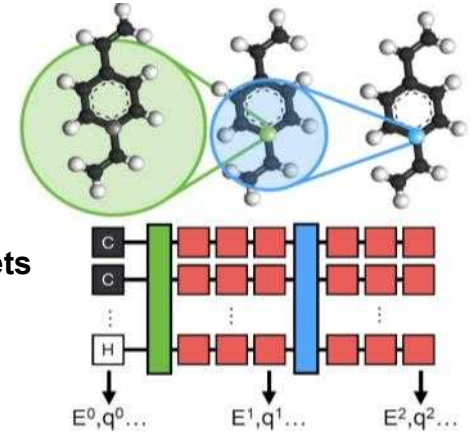
• 2 new user projects for Spring 2017, 3 more are expected for Fall, 2017

• Funded 2018 LDRD ER project

Ben Nebgen (CINT postdoc)



Neural Nets



• Major Milestone:
"Big Data" (4Tb) public release in 2017 (database of high accuracy calculations for 20M molecules)

Machine learning for energies	Our results	Google 2017
Mean Absolute Energy Error	0.40 kcal/mol	0.43 kcal/mol

Chemical accuracy = 1kcal/mol

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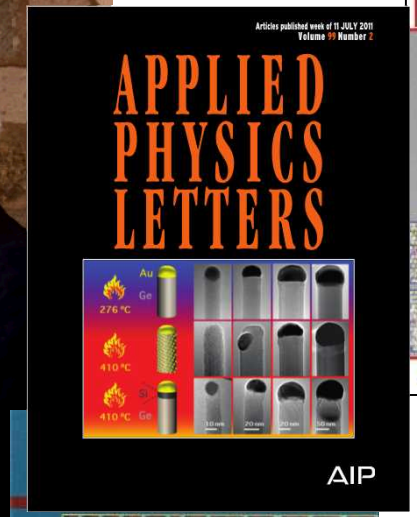
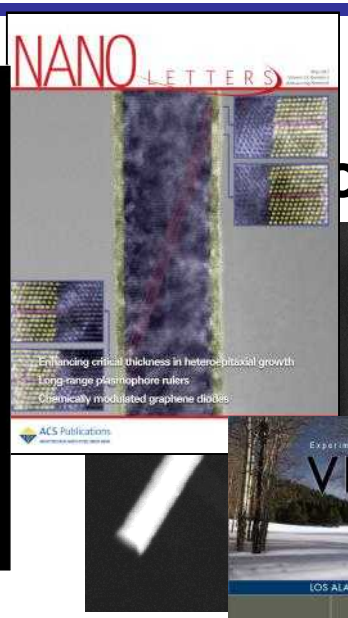
CINT User Spotlight – Shadi Dayeh

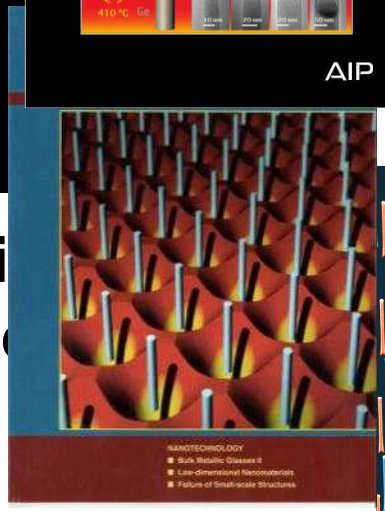
Prof. Shadi Dayeh
Department of Electrical and Computer Engineering
University of California San Diego

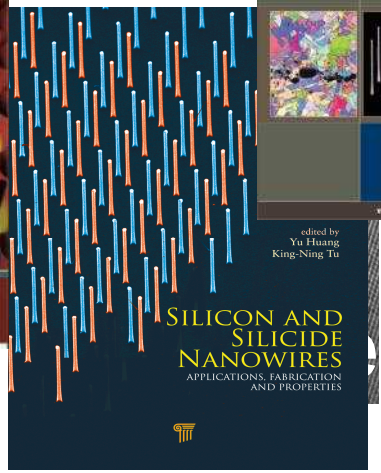
Shadi's Post Doc years at CINT

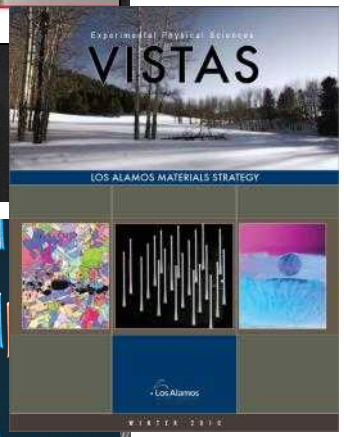
21 publications
5 Covers











IV
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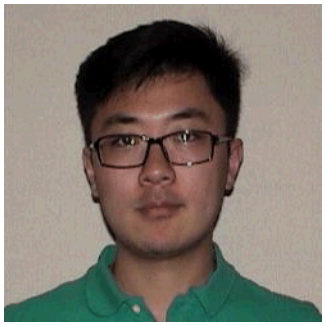
Oppenheimer Fellow worki
Tom Picraux (CINT Chief S

Shadi as a CINT User

Since becoming a professor in 2012 at University of California, San Diego



Six of Shadi's students have worked at CINT

Renjie Chen - IEEE EDS PhD Fellowship
Ren Liu - UC-National Lab In Residence Graduate Student Fellow
Xing Dai
Sang Heon Lee
Yun Goo Ro
Atsunori Tanaka

46 CINT publications since 2012!

NANO LETTERS

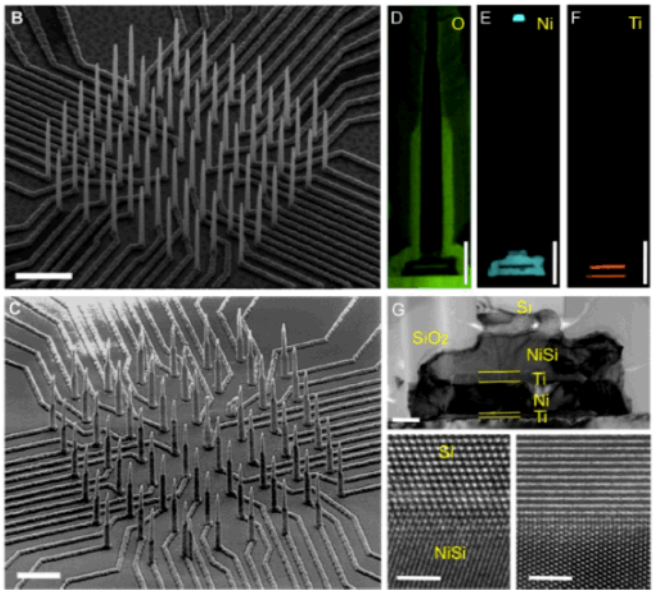
DOI: 10.1021/acs.nanolett.6b04752
Nano Lett. 2017, 17, 2757−2764 Letter
pubs.acs.org/NanoLett

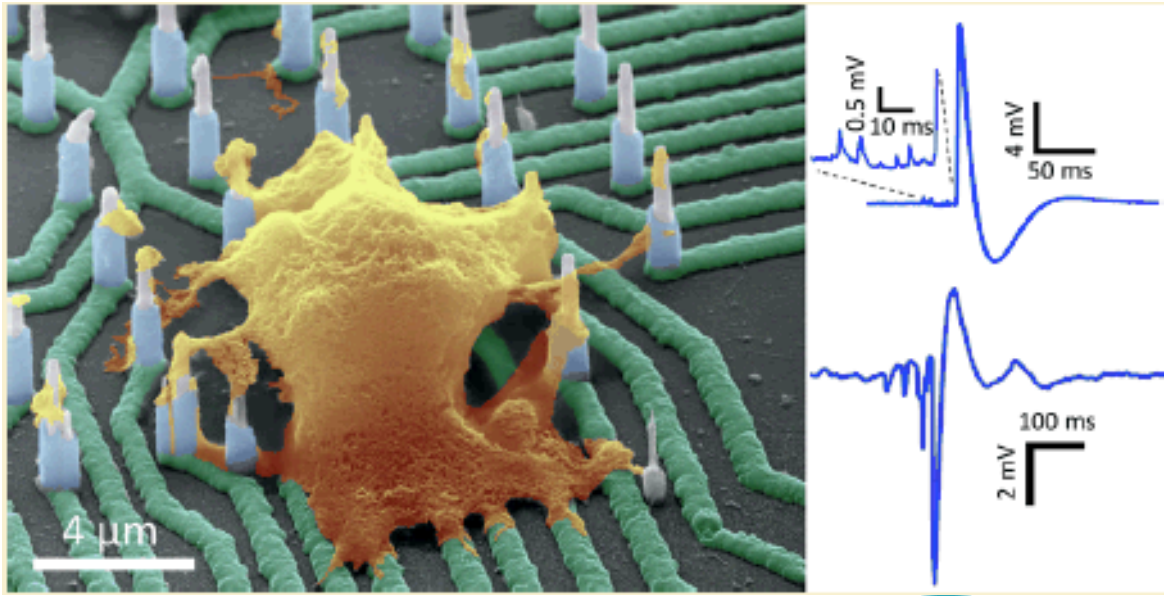
High Density Individually Addressable Nanowire Arrays Record Intracellular Activity from Primary Rodent and Human Stem Cell Derived Neurons

Ren Liu,[†] Renjie Chen,[†] Ahmed T. Elthakeb,[†] Sang Heon Lee,[†] Sandy Hinckley,[¶] Massoud L. Khraiche,[†] John Scott,[‡] Deborah Pre,[¶] Yoontae Hwang,[†] Atsunori Tanaka,[§] Yun Goo Ro,[†] Albert K. Matsushita,[§] Xing Dai,[†,#] Cesare Soci,[#] Steven Biesmans,[¶] Anthony James,[∥] John Nogan,[∥] Katherine L. Jungjohann,[∥] Douglas V. Pete,[∥] Denise B. Webb,[∥] Yimin Zou,[‡] Anne G. Bang,[¶] and Shadi A. Dayeh*[,†,§,⊥]

Use NiSi for the 1st electrically isolated vertical nanowire arrays

Measure with high sensitivity primary and stem cell neuronal activity





Shadi's UCSD Group 2017

"CINT and its facilities have helped me to contribute to the science and technology community at large.

Without the interactions with CINT, I wouldn't have advanced fast in my career, nor would have been able to pull new research directions to prosper. It also allowed me to help many postdocs and students advance in their scientific careers.

In many ways, we remain indebted to CINT. Thank you so much**."**

Shadi Dayeh

CINT User Executive Committee (UEC)

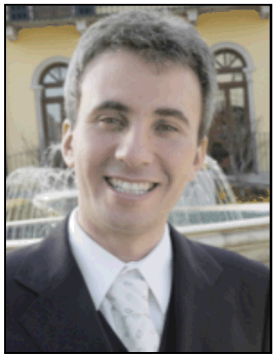
Tomorrow breakfast with UEC (7:30-9am)

Don Lucca, *Chair*
Oklahoma State University

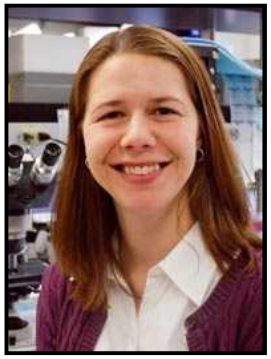
Judith Driscoll
University of Cambridge

John Grey
University of New Mexico

Karen Winey
University of Pennsylvania



Tito Busani
University of New Mexico



Diane Lidke
University of New Mexico

Erika Vreeland
Senior Scientific
Industrial Advisor

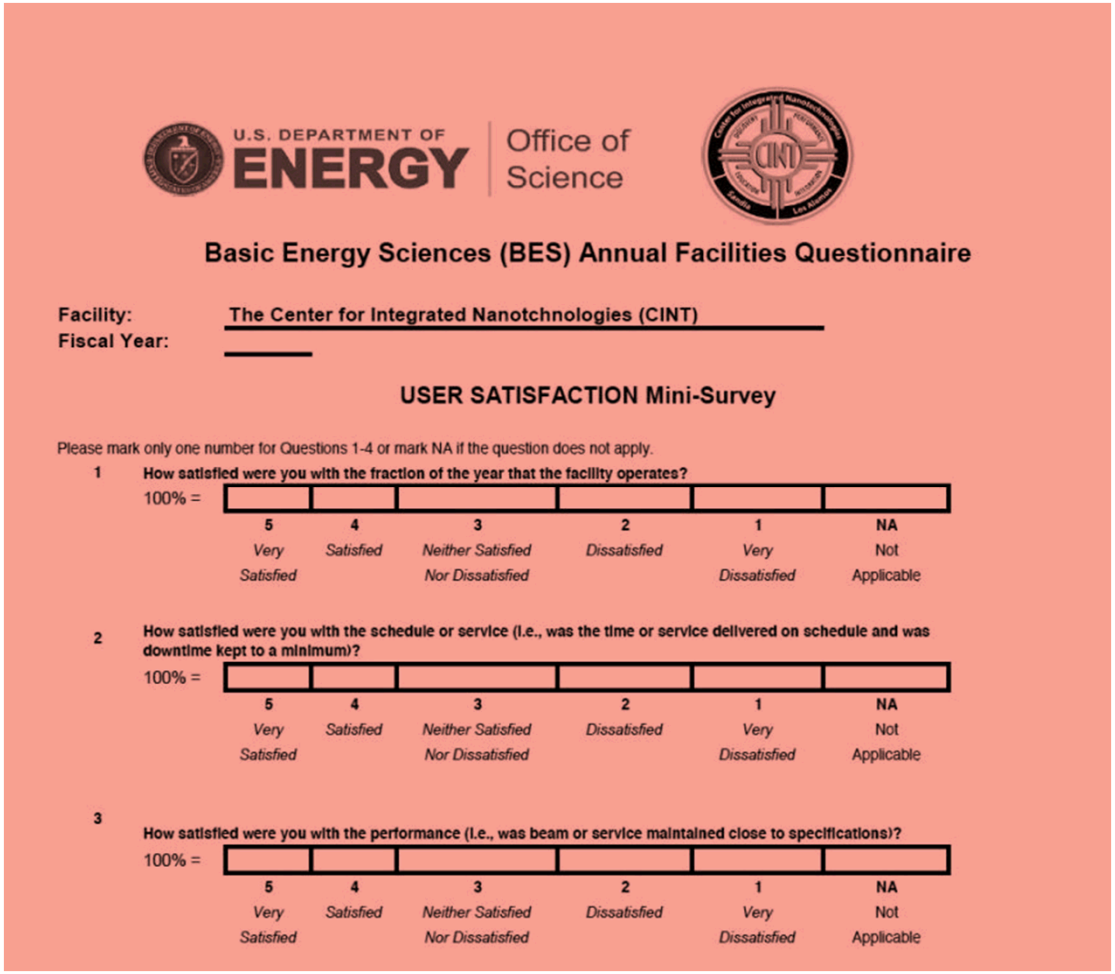
TBD
TBD
Postdoc Representative

Eric Shaner
Sandia National Laboratories
Internal Lab Representative

Dr. Don Lucca, CINT UEC Chair (lucca@okstate.edu)

Heather Brown, CINT User Program Manager (hdbrown@sandia.gov)

Please fill out the user survey



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Basic Energy Sciences (BES) Annual Facilities Questionnaire

Facility: The Center for Integrated Nanotchnologies (CINT)
Fiscal Year: _____

USER SATISFACTION Mini-Survey

Please mark only one number for Questions 1-4 or mark NA if the question does not apply.

1 **How satisfied were you with the fraction of the year that the facility operates?**

100% = | | | | | | |

5	4	3	2	1	NA
Very Satisfied	*Satisfied*	*Neither Satisfied Nor Dissatisfied*	*Dissatisfied*	*Very Dissatisfied*	Not Applicable

2 **How satisfied were you with the schedule or service (i.e., was the time or service delivered on schedule and was downtime kept to a minimum)?**

100% = | | | | | | |

5	4	3	2	1	NA
Very Satisfied	*Satisfied*	*Neither Satisfied Nor Dissatisfied*	*Dissatisfied*	*Very Dissatisfied*	Not Applicable

3 **How satisfied were you with the performance (i.e., was beam or service maintained close to specifications)?**

100% = | | | | | | |

5	4	3	2	1	NA
Very Satisfied	*Satisfied*	*Neither Satisfied Nor Dissatisfied*	*Dissatisfied*	*Very Dissatisfied*	Not Applicable