CNMS Workshop summary

CNMS Workshop on "Atom by atom fabrication with electron beams and scanning probes"

November 1-2, 2018, at Oak Ridge National Laboratory, Oak Ridge, TN

Overview: The rise of nanotechnology was heralded by the experiments conducted by Don Eigler (IBM), who used a scanning tunneling microscope (STM) tip to position xenon atoms on metal surfaces. This approach to atomic manipulation has been further developed and refined such that atomically precise engineering of materials and devices is now becoming possible. Concurrently, electron microscopy has emerged as a reliable and widespread tool, routinely offering atomically resolved images of materials. Unlike STM, electron microscopy has long been perceived as purely an imaging/characterization tool, with beam-induced modifications in the material structure considered as a hindrance to be minimized by a proper choice of imaging conditions or beam energy.

However, in the last five years, it has been demonstrated that the electron beam can induce more subtle and controllable changes in material structure, including chemical transformations of layered materials, chemical bonding between adsorbed molecules and substrates, crystallization of vacancy planes in oxides, controlled atomic dynamics of substitutional impurities and interstitial atoms, and single vacancy formation in layered materials. Combined with the development of beam control, electronics, big data acquisition and analytic tools, and AI feedback systems, this puts electron microscopy at the brink of a transition from a purely imaging tool to one capable of creating structures with atomic precision and high throughput. Once established, the field is poised for rapid growth enabled by many Scanning Transmission Electron Microscopy (STEM) platforms worldwide. Rapid realization of the opportunities enabled by electron beam and scanning probe atomic fabrication and their synergies necessitates initiating an interdisciplinary research effort combining electron and probe microscopy, data analytics/image analysis, and electrical engineering communities, as well as stringent attention to materials science aspects of these phenomena. It further necessitates the pathways and workflows for integration of the atomically-created defects with the nano- and mesoscale semiconductor and materials processing workflows, as a pathway towards the quantum computing, quantum information systems, and other fundamental and applied developments.

This workshop aimed to identify areas where atom-by-atom fabrication can provide impact on quantum devices and quantum information system and establish the synergies in collaborations between the theory, instrumentation, and experimental communities. The workshop was one of the first to bring together experts in scanning probe atomic fabrication and atomically resolved electron-beam studies to highlight recent advances and opportunities to the attention of materials research communities and serve as a much-needed seed to establish the rapid growth of the field. It further featured a range of presentations on the classical scanning tunneling microscopy-based atom-by-atom fabrication, including both atomic manipulation and integration into quantum devices that open new vistas of fundamental research. It provided a forum to present recent achievements in electron beam manipulation, novel opportunities for instrumental development enabled by the availability of high-speed data analytic tools and machine learning, discussion regarding the integration of atomic-scale device engineering in STM into semiconductor workflows, and opportunities for quantum information systems.

Workshop Outcomes: The workshop had excellent attendance: 64 registered attendees and 24 presentations. The attendees included representatives of the multiple Department of Energy (DOE) National Laboratories (Berkeley, Brookhaven, Sandia, Oak Ridge) as well as the National Institute of Standards and Technology (NIST) and the SuperSTEM laboratory, industry (Zyvex Labs), and several universities (including Harvard University, University of Oxford, Massachusetts Institute of Technology, University of Pennsylvania, and the University of Vienna). Participants included several leaders in the field, as described below, and the workshop was attended by DOE (David Forrest, Office of Energy Efficiency & Renewable Energy) and National Science Foundation (Khershed Cooper) program managers.

From the vibrant and forefront presentations and participation of the attendees, it has become clear that, a transition from the point where atomic manipulation was a *niche* application confined to a few research centers worldwide, to the point where it is becoming a practical approach for opening new opportunities in quantum materials, quantum information systems, and fundamentally new materials and devices defined on the atomic level, is now occurring. The latter, in turn, open exciting vistas into the nature of fundamental forces and interactions controlling the nano- and quantum world and opens new pathways to quantum electronic devices that are broadly perceived as an outstanding challenge for nanoscience in the coming decades.

Several common research topics and trends were identified, including:

1) The need for new tools for atomic fabrication; STM is currently perceived to be the only tool capable of direct atomic fabrication. This is the result of the early impact of STM fabrication on nanoscience as a whole, the 25+ year history of the field, and the synergy with the surface science and semiconductor workflows that allowed, after much effort, the demonstration of realistic multiple-qubit devices. Furthermore, the availability of P/Si system uniquely suited for quantum devices and knowledge of H/Si surface chemistry equip multiple scientists with the necessary fundamental knowledge.

2) Comparatively, atomic fabrication in scanning transmission electron microscopy (STEM) is a fundamentally new opportunity. The proof-of-concept experiments in the last two years performed at the University of Vienna and Oak Ridge National Laboratory are highly encouraging. However, rapid exploration and employment of these opportunities requires the delineation of the scope of material amenable to manipulation, integration into device preparation workflows (material *in vacuo* offers only limited interest), and the analysis of e-beam induced processes both on phenomenological and fundamental levels.

3) There is an emerging need for the development of *autonomous systems* using chemical or electrical energy for atomic manipulation and assembly.

4) Integration with the classical semiconductor processes is a big challenge. Much of the interest to atomically fabricated devices is driven by the opportunities in quantum physics and quantum electronics. However, creation of well-defined atomic groups is a necessary but insufficient step. This active area must to be protected and connected to the macroscopic world via classical leads or other means of information exchange.

5) Interestingly, there exists an initial market for single atom devices. While qubits and single spin magnetoelectric devices are obvious, atomically defined nanopores has excellent applications in bioelectronic, filtration, and precision sensor devices.

Key Points

- **Fundamental Science and Infrastructure:** There is considerable interest in developing single-atom or atomically defined devices in multiple areas of science, ranging from quantum computing and quantum information systems to biosensors and bioelectronics. Creating the network of practitioners and users of these capabilities, e.g., via the DOE Nanoscale Science Research Centers (NSRCs) or counterparts elsewhere in the world, can significantly accelerate the progress in these areas.

- **Integrated Tool Development:** There has been significant developments of STEMs as platforms for atomic scale manipulation. However, current microscopes generally offer a closed environment with well-packaged software/workflow that is often concealed from user control functions. Development of STEMs as a tool for atomic manipulation necessitates: (a) open software architecture allowing for the real-time detection and analytics of the detector signals for the real time feedback and the beam control, (b) significant developments on the sample preparation and transfer part avoiding contamination, etc., and (c) integration of the surface science tools (e.g., deposition) into the active region of e-beam fabrication system. The NION Swift system enables the first steps in this direction. These latter developments in some sense will integrate capabilities long common for STM systems into the STEM environment. Of interest may be the development of combined STM-STEM atomic fab tools, allowing for beam correction and visualization of STM fabricated particles and vice versa.

- **Workflows:** Fundamental scientific and technological breakthroughs in STEM-based atomic fabrication will be achieved only if the atomically fabricated devices can be integrated with the macroscopic world, ideally including the semiconductor fabrication workflow.

- **Digital Atomic Scale Fabrication.** Most nanofabrication technologies treat matter as if it is infinitely divisible and so should be considered analog fabrication. There is the opportunity both with scanning probes and electron beams to treat the making and breaking of chemical bonds as binary functions. For many of the same reasons that digital information technology has proven vastly superior to analog information technology, digital atomic scale fabrication will be able to create highly complex yet extremely reliable systems. STEMs and STMs both have necessary attributes to accomplish digital fabrication:

    - the resolution to affect a single chemical bond
    - the control of the energetics of interaction to both “read” (inspect without changing chemical bonds) and “write” (change chemical bonds),

- the spatial positioning accuracy to digitally address specific chemical bonds

For fabrication at the atomic scale, the deliberate adoption of a digital rather than the standard analog approach to fabrication will enable another digital revolution with similar advantages over the old analog approaches.

Appendix A: Program

Atom by Atom Fabrication via Electron Beams and Scanning Probes

Center for Nanophase Materials Sciences
Building 8600 Iran Thomas Auditorium

November 1-2, 2018

Thursday (November 1)

8:15 – 8:30	Bobby Sumpter (CNMS/ORNL) *Welcome and Overview*
8:30 – 9:15	John Randall (Zyvex), *Digital Atomic Scale Fabrication: Moore's Law Inverted*
9:15 – 10:00	Toma Susi (U. Vienna), *Electron-beam manipulation of graphene impurities: competing processes and modeling challenges*
10:00 – 10:30	David Forrest (DOE EERE), *Atomically Precise Manufacturing for Energy Applications*
10:30 - 11:00	*Break* – SIGN UP FOR FRIDAY TOUR – CHOOSE 1
11:00 - 11:30	Andrew L. Bleloch (Nion), *Precision control of the electron beam and the sample environment in the STEM*
11:30 – 12:00	Richard Silver (NIST), *Robust Fabrication and Measurement of Atomically Precise Devices*
12:00 – 12:15	Khershed Cooper (NSF), *NSF Nano and Advanced Manufacturing Research at NSF*
12:15 – 12:30	Benjamin Lowrie (CSED/ORNL) *Quantum photonic and phononic interactions with defects at low temperatures*
12:30 - 13:30	*Lunch and poster session*
13:30 - 14:00	Stephen Jesse (CNMS/ORNL), *Scanning Transmission Electron Microscopy for Atomic Manipulation: strategies for in-line image and spectral analysis for feedback and controls*
14:00 - 14:30	Demie Kepaptsoglou (SuperSTEM), *Single atom modification of 2D materials: fabrication and electronic structure*
14:30 - 15:00	Bethany M. Hudak (CNMS/ORNL) *Atomic-Scale Imaging and Control in the Electron Microscope*
15:00 - 15:30	*Break* – SIGN UP FOR FRIDAY TOUR – CHOOSE 1
15:30 - 16:00	Marija Drndic (UPenn), *Materials Nanosculpting and Applications*
16:30 - 17:00	Ezra Bussmann (CINT/Sandia), *Device fabrication at the atomic scale*
17:00 - 17:30	Bruno Schuler (TMF/LBNL), *Atomic-scale control and characterization of 2D materials*

Friday (November 2)

8:30 – 9:00	Prineha Narang (Harvard), *Predicting and understanding quantum defects in quantum materials*
9:00 – 9:30	Joe Lyding (UIUC) *Nanofabrication on Silicon*
9:30 – 9:45	Maxim Ziatdinov (CNMS/ORNL), *Deep learning for atomically resolved imaging: feature finding and feedback*
9:45 – 10:00	Xiahan Sang (CNMS/ORNL), *Reactions in the beam*
10:30 - 11:00	*Break*
11:00 - 11:30	Travis S. Humble (CSED/ORNL), *Atomistic Modeling and Simulation of Quantum Devices*
11:30 – 12:00	Jan Mol (Oxford), *Progress in graphene-based single-molecule electronics*
12:00 – 12:30	Robert Wolkow (U. Alberta), *Atomic Computational Elements Composed of Silicon Dangling Bonds*
12:30 - 13:30	*Lunch*
13:30 - 14:00	Dirk Englund (MIT), *Towards Large-Scale Artificial Atoms for Quantum*
14:00 - 14:15	Suhas Somnath (NCCS/ORNL), *Big data infrastrucutre at ORNL*
14:15 - 14:45	An-Ping Li (CNMS/ORNL) *Atomic scale manipulation and in situ characterization with scanning tunneling microscope*
14:45 - 15:00	David Lingerfelt (CNMS/ORNL), *Electronic excitations from electron beam irradiation and their role in atomic scale material manipulations*
15:00 - 15:30	Fernando E. Camino (CFN/BNL), *Single-Digit Nanometer Electron-Beam Lithography with an Aberration-Corrected Scanning Transmission Electron Microscope*
15:45 – 16:30	TOURS

Abbreviations

BNL: Brookhaven National Laboratory
CFN: Center for Functional Nanomaterials
CNMS: Center for Nanophase Materials Sciences
CSED: Computational Sciences and Engineering Division
DOE: Department of Energy
EERE: Office of Energy Efficiency and Renewable Energy
LBNL: Lawrence Berkeley National Laboratory
MIT: Massachusetts Institute of Technology
NCCS: National Center for Computational Sciences
NSF: National Science Foundation
ORNL: Oak Ridge National Laboratory
SNL: Sandia National Laboratories
TMF: The Molecular Foundry
U: University
UIUC: University of Illinois at Urbana-Champaign
UPenn: University of Pennsylvania

Organizing Committee: Sergei V. Kalinin, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory; Ondrej Dyck, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Program & Abstracts

Thursday (Nov. 1)

8:15 – 8:30 Bobby Sumpter (ORNL) *Welcome*
8:30 – 9:15 John Randall (Zyvex)

Digital Atomic-Scale Fabrication

John N. Randall
Zyvex Labs, Richardson Texas

Digital Information Technology, once it replaced our analog information technology, dramatically reshaped the world by providing an unbelievably complex and yet amazingly reliable set of information processing systems. I believe that nanotechnology is currently at a comparable stage as information technology was when the majority of information processing was analog. Today the promises of nanotechnology are largely unfulfilled, but that will change with a 2nd Digital Revolution: **Digital Atomic Scale Fabrication**. For many of the reasons that Digital IT is vastly superior to analog IT, digital fab will prove to be remarkably better than analog fab. The biggest advantage of digital IT is the same advantage that will fulfill the promises of nanotechnology: the ability to do error detection and correction. In nanofabrication, the digital events are the making and breaking of chemical bonds.

Zyvex Labs has been developing Hydrogen Depassivation Lithography (HDL) as a digital process. HDL is carried out with modified Scanning Tunneling Microscope (STM) instrumentation and uses electron stimulated desorption of H atoms from a Si (100) 2x1 H passivated surface. It is a form of low energy e-beam lithography. The process inherently has some digital aspects: 1) the resist (the H atoms) have a digital response, the Si-H bond is either broken or it is not. 2) The resist distribution is quantized with on H atom per surface Si atom in the beautifully ordered Si surface lattice. 3) There are distinct imaging (reading) and lithography (writing) modes well separated in energy. We have embraced the digital nature of this process to capitalize on the many advantages of digital processes.

We believe that there is a spectacular opportunity to learn from the tactics employed in information technology by Richard Hamming and many others that learned to deal with the inevitable errors in computation, transmission, and storage. This was accomplished by a host of error detection and error correction schemes. The current and rapidly evolving IT systems are incredibly complex and yet extremely reliable. We believe that by embracing and developing digital tactics with our nanofabrication processes, similarly impressive nanosystems that are not restricted to information processing will emerge.

Our ultimate goal at Zyvex Labs is the development of Atomically Precise Manufacturing where inevitable fabrication errors are detected and corrected. This technology will provide the nano-foundries required to produce the large array of nanotechnology products that have been promised but not yet delivered. I am describing a particular approach to nanofabrication, I believe that error detection/correction schemes can and will be developed in other atomic scale fabrication processes. We believe that this concept is adaptable to many other nanofabrication approaches both top down and bottom-up. **We are looking for other nanofabricators to join us in ushering in a new digital revolution.** We only need to look to the nanofabrication done in biology, to see that error detection processes are plentiful. I believe that the concept of digital

atomic scale fabrication that uses error detection and correction is not only a sound idea, it is inevitable. We are knocking on the door. **It is time for nanofabrication to go digital.**

9:15 – 10:00 Toma Susi (U. Vienna)

Electron-beam manipulation of graphene impurities: competing processes and modeling challenges

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Scanning transmission electron microscopy is emerging as fundamentally new tool for the direct assembly of nanostructures, with the ability to manipulate strong covalent bonds. Atomically precise manipulation relies on advances in instrumentation that have enabled non-destructive atomic-resolution imaging at lower electron energies. While momentum transfer from highly energetic electrons often leads to atom ejection, interesting dynamics can be induced when the transferable kinetic energies are comparable to bond strengths in the material [1]. Operating in this regime, recent experiments have revealed the potential for single-atom manipulation of Si heteroatoms in the graphene lattice using the Ångström-sized electron beam [2], with a manipulation rate comparable to state-of-the-art in fully automated scanning tunneling microscopy [3].

Evaluating the full range of future possibilities for this method requires a precise physical understanding of the interactions of relativistic electrons with various materials. For pristine graphene, excellent agreement has been obtained between experimental damage rates and displacement cross sections derived entirely from first principles [4]. However, the same does not hold for graphene impurities, where discrepancies between 10–30% in threshold energy, corresponding to several orders of magnitude in probability, are found in the best available data [5]. In addition to possible inaccuracies in the simulated threshold energies and any possible role for inelastic scattering in these impurity systems, we have recently uncovered potential competing processes, including a Stone-Wales transformation of a nearby C–C bond [3] and the orientation of the Si impurity with respect to the electron beam [6], which may affect the experimentally determined damage cross sections.

[1] T. Susi *et al.*, Phys. Rev. Lett. 113, 115501 (2014)
[2] T. Susi *et al.*, Ultramicroscopy 180, 163 (2017)
[3] M. Tripathi *et al.*, Nano Letters 18, 5319 (2018)
[4] T. Susi *et al.*, Nat. Commun. 7:13040 (2016)
[5] T. Susi *et al.*, 2D Materials 4, 021013 (2017)
[6] C. Hofer *et al.*, arXiv:1809.08946 (2018)

10.00 – 10.30 David Forrest (DOE EERE)

Atomically Precise Manufacturing for Energy Applications

David R. Forrest, ScD, PE, FASM
Technology Manager, Advanced Manufacturing Office

Atomically Precise Manufacturing (APM) refers to newly emerging capabilities to produce materials and devices that are virtually defect-free. These products will provide game-changing advances in energy applications and beyond. The presentation will describe the Dept. of Energy Advanced Manufacturing Office programming in this technology space, and the projects that are being funded. Approaches include self-assembly of engineered molecular building blocks, positional assembly using scanning probe microscopes, and positional assembly using molecular machine systems. The qualitative differences between APM and conventional technologies such as atomic layer deposition and single crystal growth (which are not atomically precise) will be discussed.

10:30 - 11:00 *Break*
11:00 - 11:30 Andrew L. Bleloch (Nion),

Instrumentation for atom-by-atom sample manipulation using an electron beam

Andrew L. Bleloch, Niklas Dellby, Tracy C. Lovejoy and Ondrej L. Krivanek
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Atom by atom manipulation by electron probes has been done both in monolayer 2D and thin 3D materials. An example of the former is moving silicon dopant atoms in graphene [1], and an example of the latter is moving Bi dopant atoms in Si [2].
This kind of work requires an electron microscope that can:

- Form a ~100pm probe at different primary energies so that the momentum transferred to the sample atoms can be tailored to the specific system of interest while maintaining atomic resolution.
- Track single atoms reliably, using a stable sample stage.
- Rapidly change the beam dwell time per pixel from <1 μs to 1 s or more, and change between different scan areas.
- Blank the beam rapidly (<1 μs).
- Change the sample temperature (from ~80K to ~1000K).
- Characterize the sample electrically without removing it from the electron microscope.
- Change the beam voltage so that the instrument mode can be changed from invasive manipulation to non-invasive imaging.
- Automatically change the microscope settings, typically in response to observed changes in the sample, guided by customized software.

All of the above tasks can be accomplished in a standard Nion microscope. Challenges of course remain, e.g., how to reliably move atoms in the direction of the beam in a 3D crystal, and how to connect fabricated nanodevices to the outside world. This talk will review the experimental capabilities already available, and discuss future possibilities.

References

[1] O. Dyck, S. Kim, E. Jimenez-Izal, A. N. Alexandrova, S. V. Kalinin, S. Jesse, *Small* 2018, 14, 1801771. DOI:10.1002/smll.201801771
[2] B. M. Hudak, J. Song, H. Sims, M. C. Troparevsky, T. S. Humble, S. T. Pantelides, P. C. Snijders, and A. R. Lupini, *ACS Nano* 2018 12 (6), 5873-5879. DOI: 10.1021/acsnano.8b02001

11:30 – 12:00 Richard Silver (NIST)

Robust Fabrication and Measurement of Atomically Precise Devices

Richard Silver
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NIST has a major program to develop atomically precise, atom-based electronic devices for use in quantum information processing, quantum materials research and quantum sensing. We are using hydrogen-based scanning probe lithography to enable deterministic placement of individual dopant atoms with atomically aligned contacts and gates to build single electron transistors and devices which display quantum behavior. We have developed robust lithography, device relocation, and contact processes that enable the routine electrical measurement and operation of atomically precise devices, with an emphasis on minimizing process-induced dopant movement.

In addition to our fabrication technology, this presentation will cover measurements of STM patterned test structures and few-nanometer scale wire devices to investigate low dimensional transport and materials properties. We will present the characterization of reproducible atomic-scale tunnel junctions and single electron transistors that demonstrate stable coulomb blockade oscillations. We will demonstrate controlled variation in electronic and quantum properties as a function of atomic scale changes in device geometry. Our low temperature measurements demonstrate superb charge stability with minimal switching events.

Our research is focused on the design and fabrication of QIP devices and emerging 2D quantum metamaterials with specific attention to atomically precise dopant placement and robust processes that yield reproducible atom-scale geometrical configurations.

This research is funded in part by the Department of Energy and by a NIST Innovations in Measurement Science award.

12:00 – 12:15 Khershed Cooper (NSF)

Nano and Advanced Manufacturing Research at NSF

Khershed Cooper, NSF

NSF's new Advanced Manufacturing (AM) program is an amalgam of previous programs that explored nano-scale, additive or subtractive manufacturing, manufacturing machines or materials engineering or cybermanufacturing. The AM program seeks new ideas in, across and outside these domain areas. Nanomanufacturing (NM) is an important component of the AM program. NM encompasses a range of diverse methods and techniques, one of them being atomically precise nanomanufacturing. In this presentation, the AM program's intent and nanomanufacturing's role within it are described, especially top-down and bottom-up approaches for atomic precision.

12:15 – 12:30 Benjamin Lawrie (ORNL)

Quantum photonic and phononic interactions with defects at low temperatures

The quantum state of photons or phonons generated by individual or coupled quantum emitters in photonic or phononic cavities is a topic of increasing interest for integrated quantum technologies. I will discuss recent measures of spectrally resolved photon correlation functions for diamond and hBN defects and the implications of those measurements for the control of single photon sources for visible to microwave wavelengths. ORNL's new investments in low temperature SEM-cathodoluminescence spectroscopy and mK optical and scanning probe microscopy with tunable magnetic, microwave and optical fields will enable a significant expansion of these efforts at ORNL. In particular, I will discuss the potential for hyperspectral imaging of the purity and indistinguishability of photonic and phononic quantum states across flexible parameter spaces.

12:30 - 13:30 *Lunch and Poster Session*

13:30 - 14:00 Stephen Jesse (ORNL),

Towards Building and Testing Quantum Structures Atom-by-Atom by Electron Beams

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Fabrication of atomic scale structures remains the ultimate goal of nanotechnology. Scanning Probe Microscopes and molecular self-assembly have demonstrated important successes towards achieving this goal. In this presentation, I discuss research activity towards the use of the atomically focused beam of a scanning transmission electron microscope (STEM) to control and direct matter on the atomic scale. Traditionally, STEM's are perceived only as imaging tools and beam induced modifications as undesirable beam damage. Our team and several groups worldwide have demonstrated that beam induced modifications can be more precise and applications more expansive. We have demonstrated ordering of oxygen vacancies, single defect and dopant formation and modification in 2D materials, and beam induced migration of single interstitials through lattices. What is remarkable is that these changes often involve one atom or small group of atoms and can be monitored real-time with atomic resolution. I will introduce several examples of beam-induced fabrication on the atomic level, and demonstrate how beam control, rapid image analytics based on traditional and artificial intelligence techniques, better insight through modelling, and image- and spectroscopy-based feedback allows for controlling matter on atomic level and investigating emergent properties.

14:00 - 14:30 Demie Kepaptsoglou (SuperSTEM)

Single atom modification of 2D materials: fabrication and electronic structure

Demie Kepaptsoglou, Fredrik Hage, Quentin Ramasse, SuperSTEM, UK
Toma Susi, Jani Kotakoski, Jannik Meyer, University of Vienna, Austria
Yung-Chang Lin, Kazu Suenaga, AIST, Japan
Trevor P. Hardcastle, Che R. Seabourne, Rik M. D. Brydson, Andrew J. Scott, University of Leeds, UK
Ursel Bangert, University of Limerick, Ireland
Julian Alexander Amani, Hans Hofsass, Universität Göttingen, Germany

The past decade has seen incredible progress in the ability to isolate and manipulate two-dimensional crystals. Due to their unique structure and dimensionality, it is possible to confine charge carriers in two dimensions, resulting in peculiar physical, chemical, and electronic properties. Such novel properties can be controlled and tuned through defects such as single atom dopants, step edges, interfaces, etc. This defect engineering takes place quite literally at the atomic level, where a combination of low voltage STEM, EELS and *ab-initio* calculations provides arguably the most powerful means of characterization. This approach was recently used to demonstrate unambiguously that low energy ion implantation can be successfully implemented to introduce single substitutional defects with excellent retention rates. The fully atomically-resolved EELS experimental data not only reveals the unique bonding signature of the dopants themselves but also their impact on the lattice surrounding them, with clear modifications observed in neighboring C atoms. Ab initio calculations are in excellent agreement with the experiment and thus not only confirm the nature of the excited states being probed by the EELS experiments but also the electronic structure reconfiguration of the doped material around the single atom dopants. Crucially, results directly confirm the possibility of tailoring the plasmonic properties of graphene in the ultraviolet waveband at the atomic scale, a crucial step in the quest for utilizing graphene's properties toward the development of plasmonic and optoelectronic devices operating at ultraviolet frequencies. These 'gentle' STEM observation conditions can nevertheless be used to drive the diffusion of substitutional dopants through single layer graphene, one atomic jump at a time. These results demonstrate that scanning transmission electron microscopy (STEM) is can emerge as an alternative method for the direct assembly of nanostructures.

SuperSTEM is the UK National Facility of Advanced Electron Microscopy funded by the Engineering and Physical Sciences Research Council (EPSRC)

14:30 - 15:00 Bethany M. Hudak (ORNL)

Atomic-Scale Imaging and Control in the Electron Microscope

Bethany M. Hudak[1], Stephen Jesse[1,2], Hunter Sims[3,4], M. Claudia Troparevsky[3], Jiaming Song[3], Paul C. Snijders[3,5], Sokrates T. Pantelides[4], Sergei V. Kalinin[1,2], and Andrew R. Lupini[1,2]

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Precise control of matter on the atomic scale is necessary for ever-shrinking devices that rely on quantum effects. The scanning transmission electron microscope (STEM) is a powerful tool for studying solid materials on the atomic scale through sub-Ångstrom-resolution imaging and spectroscopy. In recent years, these powerful microscopes have begun to pivot from purely imaging instruments to instruments that can interact with and manipulate matter. Through the deeper understanding of "damage" mechanisms in the STEM, these microscopes are increasingly being recognized as tools for atom-by-atom device fabrication. The STEM offers real-time imaging at room temperature conditions that can be paired with computer controls and feedback for precise material manipulation. Here I will discuss one way in which STEM is used to study and facilitate atomistic changes in silicon.

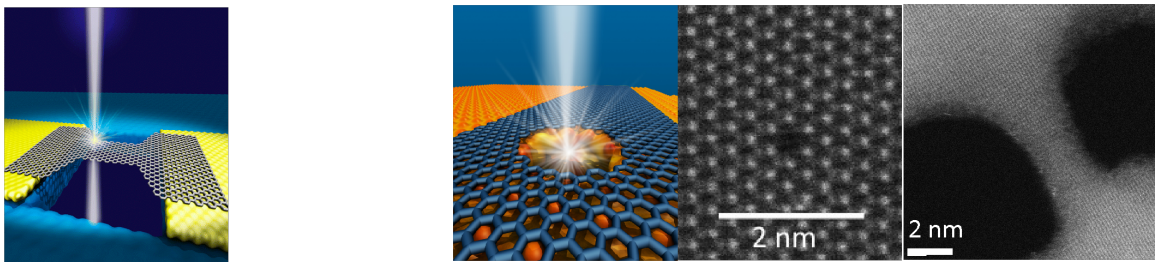
Silicon is arguably the most important technological semiconductor. Two major challenges for fabrication of quantum devices is the ability to control semiconductor growth on the nanoscale and accurately position functional subsurface dopants. Using the atomically-precise electron beam, we are able to sculpt silicon on the nanoscale. Through control of the electron beam current, we can crystallize, amorphize, and remove material entirely. In addition to Si sculpting, we also demonstrate the ability to reposition fronts of dopant atoms as well as individually position single subsurface dopants. With the real-time monitoring afforded by STEM, device architectures can be grown and edited *in situ* at the atomic scale, providing an important step toward fabrication of atomic-scale devices. These atomic-scale fabrication techniques suggest enormous potential to shape technologically important materials.

15:00 - 15:30 *Break*
15:30 - 16:00 Marija Drndic (UPenn)

Materials Nanosculpting and Applications

Marija Drndic, University of Pennsylvania

Particle beams constitute powerful tools to modify materials with atomic resolution. I will describe experiments where we push the limits of device size to atomic scale in thin materials from silicon to graphene, metal dichalcogenides and phosphorene, and expand their function and precision. Experiments include fabrication of nanoribbons and field-effect-transistors from two-dimensional materials down to sub-nm widths, and *in situ* electrical measurements including resistance vs. width for nanoribbons with different atomic structure, determining the effects of electron irradiation dose and current annealing on defect creation and healing, and the change in electrical resistance. When these experiments are combined with Raman spectroscopy, the Raman peak shifts can be used as a quantitative diagnostic tool to characterize defect density. Particle beams are also tools to punch holes in materials towards ultrafast, all-electronic analysis of molecules by driving them through tiny holes – or pores – in thin membranes. Pores whose diameters, compositions and functions we are trying to control, can detect, count, filter and analyze different kinds of ions, molecules and nanoparticles. For example, pores can quickly quantify the charge and shape of nanoparticles, or they could be used as subzeptoliter mixing volumes for nanoparticle synthesis.



From left to right: Illustrations of nanoribbon sculpting with the electron beam; passage of a DNA molecule through a Si nanopore; illustration of nanopore drilling with an electron beam inside of the TEM; one-atom-large nanopore in a MoS_2 sheet; armchair phosphorene nanoribbon sculpted in the TEM.

Selected references: Danda *et al*., ACS Nano 11 (2), 1937, 2017; Shekar *et al*., Nano Letters 16 (7), 4483, 2016, Masih Das *et al*., ACS Nano 10 (6), 5687, 2016; Rodriguez-Manzo *et al*., ACS Nano 10 (4), 4004, 2016 & ACS Nano 9 (6), 6555, 2015; Parkin *et al*., ACS Nano 10 (4), 4134, 2016; Qi *et al.,* ACS Nano 9(4), 3510, 2015; Balan *et al.*, Nano Letters 14 (12), 7215, 2015; Balan *et al*., Scientific Reports 5, 17775, 2015; Puster *et al*., Small, 22 (47), 6309, 2015; Drndic, Nature Nanotechnology 9, 743, 2014; Qi *et al.*, Nano Letters 14 (8), 4238, 2014; Rosenstein *et al*., Nature Methods, 9 (5), 487, 2012.

16:30 - 17:00 Ezra Bussmann (Sandia)

Device fabrication at the atomic scale

Ezra Bussmann
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Atomic precision advanced manufacturing (APAM) techniques via scanning probe methods are a prescient tool to study materials and device engineering with controlled few-atom defects and inherently quantum mechanical behavior. This talk describes some advantages, challenges, recent advances, and opportunities for atomic precision manufacturing of electronic materials and devices via scanning probe microscopy. Our recent success mitigating some contemporary materials and manufacturing challenges, e.g. integrating APAM material into efficient Si foundry style processes, is being leveraged to make electronic devices for analog quantum simulation and tests of beyond-Moores digital device concepts.

This work was supported by the Laboratory Directed Research and Development Program at Sandia National Laboratories, and was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. Department of Energy (DOE), Office of Basic Energy Sciences user facility. Sandia National Labs is managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government.

17:00 - 17:30 Bruno Schuler (Molecular Foundry)

Atomic-scale control and characterization of 2D materials

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Layer-by-layer control in the synthesis and processing of new materials has emerged as an important materials science challenge for future quantum devices. Particularly the advent of van der Waals materials has attracted considerable attention in this respect because of the intrinsic anisotropy in their lattice structure.

Here we give an overview of two selective and self-limiting processes to add or remove atomic layers applicable to both van der Waals and conventional solids. Specifically, we used atomic layer deposition (ALD) to grow 2D transition metal dichalcogenides (TMDs) on a wafer scale. Atomic layer etching (ALE) was used to remove SiO_2 layers with sub-nm precision.

Furthermore, we will discuss how we can characterize low-dimensional material systems using a suite of high-resolution characterization tools available at the Molecular Foundry, such as scanning tunneling and atomic force microscopy, transmission electron microscopy (at NCEM), near-field optical microscopy, angle-resolved photoemission spectroscopy (at ALS) and cathodoluminescence microscopy.

In particular, we identified and characterized point defects in CVD-grown monolayer WS_2 using low-temperature scanning probe microscopy with CO functionalized tips. We found that both the intrinsic Cr_W substitute as well as the annealing-induced S vacancy feature deep spin-orbit split defect orbitals. The atomic-scale characterization and control of defects in 2D materials is critical as they affect the materials properties beyond conventional doping in semiconductors.

Friday (Nov. 2)

8:30 – 9:00 Prineha Narang (Harvard)

Predicting and understanding quantum defects in quantum materials.

Today, we imagine a world where we can engineer materials and devices atom-by-atom. Exciting discoveries during the past few decades in quantum science and technology have brought us to this next step in the quantum revolution: the ability to fabricate, image and measure materials and their properties at the level of single atoms is almost within our grasp. Yet, at the most fundamental level a tractable quantum mechanical description and understanding of these materials does not exist. The physics of quantum materials is rich with spectacular excited-state and non-equilibrium effects, but many of these phenomena remain poorly understood and consequently technologically unexplored. Therefore, my research focuses on understanding how quantum-engineered materials behave, particularly away from equilibrium, and how we can harness these effects for quantum technologies. I will present my approach, from a theoretical and computational standpoint, in this talk. Electron-photon, electron-electron as well as electron-phonon dynamics and far-from-equilibrium transport are critical to describe ultrafast and

excited-state interactions in materials. *Ab initio* descriptions of phonons are essential to capture both excitation and loss (decoherence) mechanisms, and are challenging to incorporate directly in calculations due to a large mismatch in energy scales between electrons and phonons. I will show results using a new theoretical method we have developed to calculate arbitrary electron-phonon and electron-optical interactions in a diagrammatic many-body framework integrated with a non-equilibrium carrier transport method. Further, I will discuss a new formalism at the intersection of cavity quantum-electrodynamics and electronic structure methods, quantum-electrodynamical density functional theory (QEDFT), to treat electrons and photons on the same quantized footing. I will demonstrate how these *ab initio* techniques can guide the search for relevant quantum properties in 2D and 3D materials, including new quantum emitters.

9:00 – 9:30 Joe Lyding (UIUC)

Nanofabrication on Silicon

No abstract.

9:30 – 9:45 Maxim Ziatdinov (ORNL)
Deep learning for atomically resolved imaging: feature finding and feedback

Maxim Ziatdinov (CSED ORNL)

We demonstrate a number of approaches based on deep neural networks for automated analysis of static and dynamic electron and scanning probe microscopy data. Deep neural networks trained on theoretical and/or small amount of experimental data allowed a rapid access to the atomic degrees of freedom in noisy static and dynamic experimental data, which was not possible to achieve with previously known methods. We demonstrated their successful applications for creating libraries of atomic defects, analyzing structural phase transformations under electron beam irradiation and mapping chemical transformation pathways on the atomic level.

9:45 – 10:00 Xiahan Sang (ORNL)

Reactions in the beam

In this talk, I will show how *in situ* STEM is used to investigate the dynamics of 2D material reconstruction and growth at atomic resolution at elevated temperature accelerated by electron beam irradiation. Edge evolution of nanopores in $Mo_{1-x}W_xSe_2$ monolayers was investigated via atomic-resolution *in situ* STEM and these edges are structurally transformed to theoretically predicted metastable atomic configurations by thermal and chemical driving forces. The coupling of predictive modeling and *in situ* STEM imaging in evolving chemical environments demonstrated here provides a pathway for the controlled atomic scale manipulation of matter for

the directed synthesis of edge configurations in $Mo_{1-x}W_xSe_2$ to achieve desired functionality. Also, this approach was used to provide direct insight into the homoepitaxial Frank-van der Merwe atomic layer growth mechanism and here we demonstrate how the process can be exploited to obtain new transition metal carbides (TMC) phases that is synthesized on surfaces of Ti_3C_2 MXene substrates with the substrate being the source material. This work could lead to the development of novel bottom-up synthesis methods, such as CVD and MBE, for controllable synthesis of larger-scale and higher quality single-layer TMC.

10:30 - 11:00 *Break*
11:00 - 11:30 Travis Humble (ORNL)

Atomistic Modeling and Simulation of Quantum Devices

Travis S. Humble, Oak Ridge National Laboratory

Fabrication and control of individual atoms, electrons, and photons are the basis for a broad variety of quantum computing technologies. Robust quantum devices will require very accurate and precise engineering of the atomic, molecular, and optical states. In this talk, we discuss the interplay in material defects and control signals for doped silicon quantum devices design. We couple electrostatic device calculations with electronic structure calculations of the silicon dopant. We observe significant differences in the expected operation of the device depending on the level of materials theory used, including a concentration of spin amplitude at the dopant site. This impacts the requirements on fabrication precision as well as the required field parameters.

11:30 – 12:00 Jan Mol (Oxford)

Progress in graphene-based single-molecule electronics

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Five years ago we began to investigate the use of graphene nanoelectrodes for contacting individual molecules [1] and recently we began to translate this platform to a suspended TEM-compatible architecture. Graphene nanoelectrodes allow for non-covalent bonding of molecules [2], effective electrostatic gating, large-scale fabrication [3], atomic manipulation [4], and integration with other nano-electronic components [6]. The great success of this approach is only lessened by the fact that, unlike in the case of gold nanoelectrodes, graphene nanoelectrodes cannot simply be thought of as ideal, semi-infinite metal leads [6]. As the electronic and thermal properties of the graphene nanoelectrodes significantly influence the behaviour of the graphene-based single-molecule devices, the atomistic details of the graphene-molecule-graphene junction needs to be considered as a whole. Here, I will present a broad overview of the challenges and progress in understanding and controlling the interactions between individual molecules anchored to graphene nanoelectrodes and their environment and how these lessons can translate to emerging experiments manipulating atoms on the atomic scale in graphene and other 2D materials. I will focus on the influence of the unique material properties of graphene – its two-dimensional nature, electronic band structure, and long mean-free path – have on potential single-molecule device applications such as transistors [7], heat engines [5], and sensors [8].

Additionally, I will offer some initial thoughts on the prospects for translating these findings to covalent architectures along with requirements for studying the quantum transport in cryogenic environments.

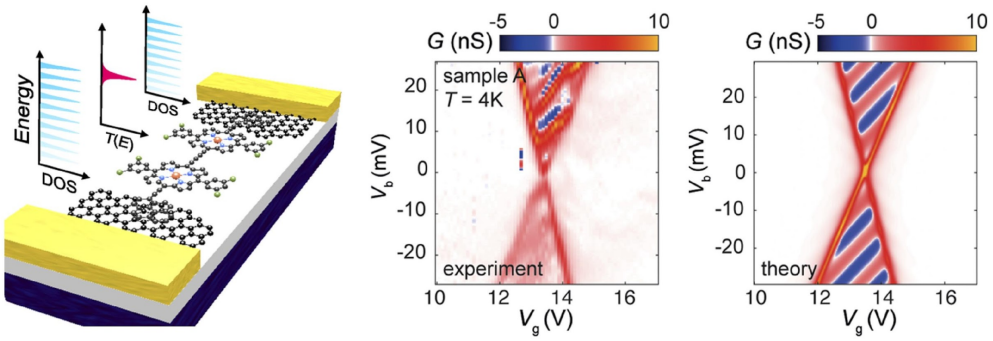

Figure 1 : The influence of the electronic structure of graphene nanoelectrodes on the sequential electron tunnelling in a single-molecule transistor.

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[8] P. Puczkarski et al., Low-Frequency Noise in Graphene Tunnel Junctions, ACS Nano 12, 9451 (2018)

12:00 – 12:30 Robert Wolkow (U. Alberta)

Atomic Computational Elements Composed of Silicon Dangling Bonds

Robert Wolkow
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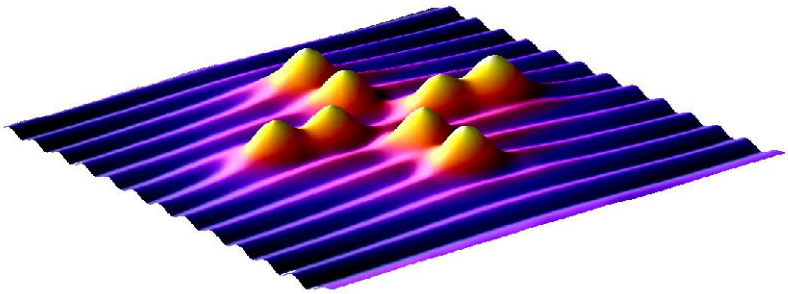
Atomic circuitry composed of silicon surface dangling bonds have the potential to address the shortcomings of CMOS. Single dangling bonds behave as atomic silicon quantum dots, in part because such states (and ensembles of such states) are in the band gap and mix poorly with continuum bulk states. Our circuitry appears to have several attractive properties:
Consumes far less energy than CMOS; extreme clocking/THz; ultra compact, low mass; all dots are identical; all distances among dots in an ensemble are identical (rendering all ensembles identical); simple and "green" processing – in one step all active and passive components printed - no layers or mask alignment; can be merged on same chip with CMOS; can perform classical binary logic (proven), likely can perform quantum operations (modeled, yet to be tested), and perhaps most excitingly, can be deployed in entirely unique ways.
An example of a unique application of the atomic silicon circuitry will be described. Paired dots form

a double well potential occupied by one electron. Nearby charges can bias a double well potential to give a preferred occupation of one side of the double well. Multiple pairs and fixed charges have been positioned to create an ensemble that can be viewed as a model – *actually a simulator* – of a nano-magnet. Such a system is the physical embodiment of an Ising model Hamiltonian. Rather than calculating the properties of such an entity, we merely read them. Because we can read out the state of each bit (the electron position in each atom pair) we can trivially collect a Boltzmann distribution – that is – the fluctuations in energy of this "machine" as it experiences thermal buffeting by the environment.

As we can build an atomic electronic entity that is isomorphous with a neural network, we can foresee ways to more rapidly and accurately achieve unsupervised machine learning. Plans for couplers allowing controlled interaction without physical proximity will be touched upon as will options for exploring quantum behavior. Perfect, atom-defined SETs will enable rapid readout (no microscope will be required).

Lastly, machine learning has been applied to automate our scanned probe fabrication tool: without human supervision, probe errors which occasionally occur are detected and repaired allowing atom-perfect fabrication to proceed, unattended. We now see no barrier to massively parallel, perfect, atom-scale fabrication and therefore to viable, commercial products.

T. Huff et al., arXiv:1706.07427 (2017)
M. Rashidi, et al., Phys. Rev. Lett. 121, 166801 (2018)



A scanning tunneling microscope image of a hydrogen terminated silicon 100 surface on which 8 dangling bonds have been prepared by the removal of 8 hydrogen atoms. These atoms behave as atomic quantum dots and ensembles of dots can be tailored to achieve a wide range of properties. The entity shown here is a "cross", that is, a structure allowing binary signals on two orthogonal lines to pass through one another without interaction. This capability allows truly 2 dimensional circuitry (the avoidance of multilayers and vias between layers) and enhanced connectivity without going out of the plane.

12:30 - 13:30 *Lunch*

13:30 - 14:00 Dirk Englund (MIT)

Towards Arrays of Designer Artificial Atoms for Scalable Quantum Technologies

Quantum technologies are now emerging with astonishing capabilities that are unmatched by their classical counterparts, such as unconditionally secure communication, quantum computing, and quantum-enhanced sensing. The next grand challenge involves realization of large-scale quantum systems suitable

for practical real-world applications. To attain this challenge, it will be necessary to develop advanced theoretical methods for quantitative prediction of quantum defects, the production and imaging of single and arrayed solid-state quantum systems with nanoscale precision, and quantum control techniques to coherently initialize, control, and measure complex solid-state quantum systems. This talk will in particular consider atom-like emitters in diamond and in emerging 2D materials, where
diamond enables exceptional coherence properties and 2D materials offer a “quantum canvass” for inducing and imaging quantum defects.

Bio: Dirk Englund received his BS in Physics from Caltech in 2002. Following a year at TU Eindhoven as a Fulbright Fellow, he earned his MS in EE and PhD in Applied Physics from Stanford University in 2008. He was a postdoctoral fellow at Harvard University until 2010, when he became Assistant Professor of E.E. and Applied Physics at Columbia University. He joined the MIT EECS faculty in 2013. Recent recognitions include the 2011 PECASE, the 2011 Sloan Fellowship in Physics, the 2012 DARPA Young Faculty Award, the 2017 ACS Photonics Young Investigator Award, and the OSA's 2017 Adolph Lomb Medal.

14:00 - 14:15 Suhas Somnath (ORNL)

Big Data Infrastructure at Oak Ridge National Laboratory

Numerous scientific domains, including materials science, are undergoing profound changes, driven by increased access to high-performance computing, numerical simulations of ever larger systems, and continual improvements to instrumentation that have resulted in an explosion in the data volume, dimensionality, complexity, and variety. In addition, computer vision and machine learning have begun to transform the landscape for nearly every scientific field through recognition of patterns, extracting features, etc. that would have been overly tedious or impossible via conventional techniques. The sheer power of machine learning, the explosion in data volumes and velocity, complex sequences of data processing operations, and the computational intensiveness of algorithms have necessitated the development and deployment of software, tools, and infrastructure to accelerate data driven scientific discovery.

Oak Ridge National Laboratory (ORNL) is home to the Oak Ridge Leadership Computing Facility (OLCF) which not only houses some of the world’s fastest supercomputers like Summit and Titan but also provides several software and services for big data needs. These services include a variety of popular workflows to orchestrate complex sequences of data movement and processing operations, container frameworks to facilitate the development and deployment of portable software applications, data visualization, and scalable data analytics software. The Compute and Data Environment for Sciences (CADES) serves as an on-ramp and off-ramp for the OLCF by providing flexible cloud computing, robust data storage, scalable high performance computing, specialized compute resources for deep-learning, cross-facility integration that include the connection of experimental facilities to CADES, robust data management and transfer facilities, in addition all the services offered by the OLCF.

14:15 - 14:45 An-Ping Li (ORNL)

Atom manipulation and in situ characterization with scanning tunneling microscope

Marek Kolmer, Chuanxu Ma, Giang Nguyen, An-Ping Li

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Miniaturization of electronic circuits into the single-atom level requires novel approaches to fabrication and characterization of the atomic system. Due to its unrivalled precision scanning probe microscopy is currently regarded as the method of choice for both fabrication and characterization of atomic and molecular structures supported on surfaces. In particular, a multi-probe STM, by combining the atomic precision and resolution of STM with the real-time imaging capability of SEM, provides unprecedented opportunities to build atomic structures atom-by-atom, characterize the electronic and magnetic properties, and test fundamental quantum response as a function of controlled perturbations while the atomic system is built. Here we first describe how we use STM to image, write, and erase single vacancy defects in 2D materials, and event to direct chemical reaction for synthesizing atomic precise graphitic heterostructures. We will then focus on the application of a new generation of 4-probe STM in fabrication of nanowires with single atom in width and defined number of atoms in length on Ge(001) surface. We will introduce a novel method for the determination of the transconductance in a two-probe experimental setup and demonstrate how it captures energy-resolved coherent transport through the unoccupied surface states. Our work illustrates the capability of making, characterizing, and understanding quantum materials at the atomic precision with STM-based methods.

14:45 - 15:00 David Lingerfelt (ORNL)

Electronic excitations from electron beam irradiation and their role in atomic scale material manipulations

David Lingerfelt, Jacek Jakowski, Panchapakesan Ganesh, Bobby Sumpter

Explicitly time dependent electron structure theory methods permit the simulation of electronic dynamics in “real time” and have become prominent tools for simulating of the (potentially non-linear) response of molecular and nanoscaled materials’ to time-dependent external perturbations. Their utility for treating the response of nanoscale materials to incident electron beams will be discussed here, with emphasis on the first principles prediction of EELS spectra and EELS maps. The electric dipole approximation to the EELS intensity is scrutinized across a wide range of impact parameters for simple atomic systems, and a general method to gauge its validity is developed. The different selection rules for optical and electron beam induced electronic excitations are discussed in light of the symmetries of the involved electronic states. Future directions including Lorentz-covariant treatment of the swift electron’s scalar potential and coupling of electronic and vibrational dynamics in order to model materials transformation will also be discussed, opening to door to accurate *ab initio* simulation of state-resolved energy transfer pathways from beam electrons to materials’ electronic and nuclear degrees of freedom.

15:00 - 15:30 Ferdinand E. Camino (CFN BNL)

Single-Digit Nanometer Electron-Beam Lithography with an Aberration-Corrected Scanning Transmission Electron Microscope

Fernando E. Camino, Vitor R. Manfrinato, Aaron Stein, Lihua Zhang, Ming Lu, Eric A. Stach, and Charles T. Black
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We use an aberration-corrected scanning transmission electron microscope to define single-digit nanometer patterns in two widely-used electron-beam resists: poly (methyl methacrylate) and hydrogen silsesquioxane. Resist patterns can be replicated in target materials of choice with single-digit nanometer fidelity using liftoff, plasma etching, and resist infiltration by organometallics.

15:45 – 16:30 Tours

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