     

Joint NSRC Workshop

Big, Deep, and Smart Data Analytics in Materials Imaging

Jointly Organized by the Five DOE Office of Science Nanoscale Science Research Centers
and Held at Oak Ridge National Laboratory, Oak Ridge, TN
June 8-10, 2015
(www.cnms.ornl.gov/JointNSRC2015/)

Workshop Summary and Recommendations

Program Committee:
Eric Stach, Center for Functional Nanomaterials, Brookhaven National Laboratory
Jim Werner, Center for Integrated Nanotechnologies, Los Alamos National Laboratory
Dean Miller, Center for Nanoscale Materials, Argonne National Laboratory
Sergei Kalinin, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory
Jim Schuck, Molecular Foundry, Lawrence Berkeley National Laboratory

Local Organizing Committee:
Hans Christen, Bobby Sumpter, Amanda Zetans, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

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Understanding and ultimately designing improved functional materials that possess complex properties will require the ability to integrate and analyze data from multiple instruments designed to probe complementary ranges of space, time, and energy. Recent advances in imaging technologies have opened the floodgates of high-veracity information in the form of multidimensional data sets. These high-resolution images and spectra conceal unexamined information on atomic positions and local functionalities, as well as their evolution with time, temperature, and applied fields. To gain the full benefits of such data sets, we must be able to effectively interrogate them for a variety of physically and chemically relevant information, develop pathways for probing local structure-property relationships, and synergistically link these results to atomistic theories (e.g., deep data analysis for scientific inference). The traditional simple graphical representation and visual inspection of such data sets are no longer sufficient to extract the most meaningful information. Advanced mathematical and computational methods are increasingly being incorporated into imaging sciences to deal with such "deep" data sets, and to combine data streams from different imaging techniques. However, many of the required mathematical or numerical tools are either lacking or not generally accessible to the imaging sciences community.

The workshop "Big, deep, and smart data in materials imaging", jointly organized by the five Office of Science Nanoscale Science Research Centers (NSRCs) and held June 8-10, 2015 at Oak Ridge National Laboratory, brought together researchers from different imaging disciplines (electron microscopy, scanning probe microscopy, focused x-ray, neutron, atom probe tomography, chemical imaging, optical microscopies) as well as experts in mathematical/statistical/computational approaches to discuss opportunities and future needs in the integration of advanced data analytics and theory into imaging science. It provided a forum to present achievements in the various imaging disciplines with emphasis on acquisition, visualization, and analysis of multidimensional data sets, the corresponding approaches for theory-experiment matching, and novel opportunities for instrumental development enabled by the availability of high speed data analytic tools.

The workshop aimed to identify areas where advanced data analytics approaches will significantly increase the quality of information extracted from imaging data, and identify the role to be played by the NSRCs to make such approaches accessible to the user community. At the same time, the workshop identified areas in which enhanced interaction with researchers in applied mathematics, statistics, theoretical and computational sciences will be most beneficial to the imaging and materials sciences community in particular, and nanosciences in general.

The workshop far exceeded expectations on attendance: ~150 registered attendees, 33 presentations, ~50 posters. The attendees included representatives of the multiple DOE National Laboratories (LBNL, ANL, BNL, SNL, LANL, ORNL, Ames Lab, PNNL) as well as Frederick National Laboratory for Cancer Research, NIST, ARL, industry (Asylum, NewPath, Gatan, HP), and 16 universities (including Berkeley, MIT, UWisc, UCSD, etc.). Participants included several leaders in the field, as described below and DOE program managers (Maracas, Lee) as observers. Furthermore, several of the attendees are chairing symposia at the Fall MRS meeting in Boston along a similar direction. Overall, this indicates that the area of big, deep and smart data in materials imaging is seen as a very high priority by a broad representation in the scientific community. From the content of the presentations, it became obvious that the topic of establishing data, knowledge, and skill-set connections between imaging and HPC infrastructure is evolving very rapidly, and is not limited by the introduction of new instrumentation but rather by connection between individual efforts.

Several common research topics were identified, including

1. The need for mathematical tools for imaging, especially those based on compressed sensing (LBNL, ANL, PNNL) and Markov chain models (NIST, Purdue)
2. Opportunities with ptychography (ANL and LBL for X-ray, LBL and ORNL for STEM)
3. Development of pipelines for direct data transfer from imaging tools (STEMs/XRay/SPM) to HPC (LBL, BNL, ANL, etc)
4. Direct image quantification via atomic positions (ORNL, LBL, NCSU, NIST)
5. Beam control in STEM for fats data acquisition and matter manipulation (ORNL)

We note that the selection of these topics is driven either by the physics of the imaging process (e.g., low dose imaging necessitates compressed sensing methods) or new opportunities for characterization of matter (ptychography, which effectively combines scattering and sub-atomic resolution imaging). Pursuing these directions in turn requires the development of the infrastructure (pipelines) and data analytics tools (visualization, unsupervised learning, reconstructions), in the absence of which the amount of information available for analysis is limited by human analysis and a selection bottleneck. Also noteworthy is that many of these programs have been active for extended periods of time (CAMERA at LBL for 6 years, I^3 at Argonne for 2 years, chemical imaging initiative at PNNL for ~4 years).

Workshop overview: Smart imaging of materials lets national labs look to solving big energy problems

In the Stone, Bronze and Iron Ages, the state of the art of materials science defined the zenith of technology and accelerated economies. Now, in the Information Age, data drives the development of advanced materials for energy-efficient superconducting wires, safer nuclear power plants, stronger, lighter vehicles with better batteries—and more. In this context, this workshop discussed opportunities and challenges as imaging and data sciences merge. Those efforts will likely aid the Materials Genome Initiative, which aims to speed new materials to the global marketplace.

“Combining physics with big data could produce a new field, akin to the merger of biology and engineering that created bioengineering,” said **Sergei Kalinin**, an organizer of the workshop and director for ORNL’s Institute for Functional Imaging of Materials.

Companies like Google and Facebook have long grappled with a volume, variety and velocity of data that characterizes it as “big.” Members of the scientific community, however, have differing degrees of experience with “big data.” Physicists sifting through mountains of data from a collider experiment to find signs of an exotic subatomic particle, for example, have more experience with it than do materials scientists examining images of a failed battery material, who often cherry-pick data related to the failure but leave the rest of the data unexamined.

That unmined data may hold vast riches. To reveal them, big data approaches must get deeper and smarter. “Deep data” strategies use theory to inform experiment and vice versa. “Smart data” tactics, on the other hand, try to do those better with unparalleled expertise and equipment.

With its big-data focus, industry isn’t advancing the deep- or smart-data approaches needed to accelerate advances in materials for energy applications. “Big data means correlation, and ignores causation,” Kalinin said. A deeper, smarter approach that merges imaging data with physical laws may allow scientists to understand the causes of problems in existing materials and predict the behaviors of designed materials. But that strategy depends on directly transferring atomically-resolved data from scanning transmission electron microscopes and X-ray experiments to high-performance computing resources for analysis and visualization.

“Facebook and Google use and re-use information already on the web. Our ground floor is to build an instrumental infrastructure that can stream data to the web,” Kalinin envisioned. “Traditionally, imaging instruments were not developed to provide uninterrupted data to the web, so only small fraction gets analyzed. We need to develop data pipelines.”

Promising merger

The workshop’s speakers shared promising projects that merge imaging and data sciences. “The merger allows scientists to do something deeper, but challenges remain in bringing together two philosophies,” Kalinin said. “Data is understood numerically, but imaging is not—yet.”

A looming challenge is unifying the language of microscopic data to establish common definitions for the “information content” of images. ORNL microscopist **Albina Borisevich** said she no longer “takes pictures” of materials but instead collects ever-increasing amounts of quantitative data from them. That data provides information about material properties and structures at atomic resolution with precision approaching that of X-ray and neutron characterization tools. Engaging advanced computational approaches brings new capabilities in data analysis, such as allowing analysis of physics and chemistry reflected in picometer-level details of images. “Cross-pollination of different imaging disciplines with computational flavor is already bringing unexpected fruit,” she said. “Implementation of the scanning-probe-like beam control allows us to use electron microscopy to fabricate the smallest 3D structures.” Similar work is being performed at U. Wisc. by Paul Voyles, who have demonstrated the use of advanced image analytics tools to increase precision of atomic position in STEM to sub-pm. This work closely alignes with the effort of J. LeBeau of NCSU devoted ot experimental analysis of atomically-resolved images, and S. Patala applying the graph theory to image parametrization.

James Sethian, a mathematics professor at the University of California, Berkeley, spoke about CAMERA, a pilot project he directs at Lawrence Berkeley National Laboratory that DOE’s offices of Basic Energy Sciences (BES) and Advanced Scientific Computing Research (ASCR) support. CAMERA convenes interdisciplinary teams of mathematicians, experimental scientists and software engineers to build mathematical models and algorithms for tools critical to users of DOE facilities. “When these teams work together, they can make sense of the deluge of data, and provide the insight to turn data into information that can accelerate our scientific understanding,” he emphasized. He described work on ptychography (which combines scattering and sub-atomic resolution imaging), image analysis, chemical informatics, GISAXS (grazing-incidence small-angle X-ray scattering) and fast methods for electronic structure calculations. D. Ciston of LBL further demonstrated the use of advanced mathematical tools in the form of image libraries for fast analysis of ptychographic data in STEM.

ORNL mathematician **Rick Archibald** provided an overview of the ACUMEN project, funded by ASCR and focused on the mathematical challenges of scientists at the SNS and CNMS. To bring high-performance computing to the massive data sets generated by scientific experiments at ORNL, ACUMEN's partners develop next-generation algorithms for scalable analytics. M. Demkovicz of MIT delineated the use of Bayesian methods for analysis of the image data and reducing it to materials specific parameters.

"Powerful imaging techniques demand increasingly large bursts of computing power to drive their data analysis," said **David Skinner**, who leads strategic partnerships between the National Energy Research Scientific Computing Center (a DOE Office of Science User Facility at Lawrence Berkeley National Laboratory) and research communities, instrument/experiment data science teams and the private sector. "Accessing shared high-performance computing through fast networks is an increasingly interesting prospect for these data-driven instruments."

ORNL software engineer **Eric Lingerfelt** described the Bellerophon Environment for Analysis of Materials (BEAM) software system, which will, for the first time, enable instrument scientists at CNMS to leverage ORNL's powerful computational platform to perform near real-time data analysis of experimental data in parallel using a web-deliverable, cross-platform Java application. The BEAM system also offers robust long-term data management services and the ability to transmit data files over ORNL's high-speed network directly to CADES. "BEAM users can easily manipulate remote directories and data in their private storage area on CADES as if they were browsing their local workstation," Lingerfelt said. Similar effort is being undertaken by F. Ogletree and his team at LBL.

Managing unprecedented data streams is a big challenge. Fortunately, colocation of NSRCs with other facilities grappling with this elephantine issue gives DOE nanocenters a huge advantage in finding solutions. RHIC, an accelerator at Brookhaven National Laboratory (BNL) looking at the quark gluon plasma, and ATLAS, a detector at CERN's Large Hadron Collider, are both high-energy physics projects that generate lots of data. The RHIC & ATLAS Computing Facility at BNL manages the data for both. **Eric Stach**, who leads the Electron Microscopy Group in the Center for Functional Nanomaterials at BNL, noted that the RHIC/ATLAS detector curated 160 petabytes of data in 2013, and will surpass 200 petabytes this year. So materials scientists have learned a lot from nearby physicists—a boon because a single STEM instrument can produce a data flow similar to that of the ATLAS detector, Kalinin interjected. Said Stach, "The introduction of sensitive new detectors and ultra-bright sources is leading to an explosion of rich materials data—we expect to have more than 20 petabytes generated each year at the user facilities at Brookhaven. That's the data equivalent of one-fifth of every Google search done in 2013."

Nigel Browning of Pacific Northwest National Laboratory (PNNL) described methods, statistics and algorithms to extract information from images obtained using aberration corrected electron microscopy, which enables very high resolution images of increased data quality and quantity. Compressive sensing, for example, pays attention to bits of a sample and uses signal processing to fill in the blanks. **Kerstin Kleese van Dam,** then of PNNL (now at BNL), spoke about streaming analysis of dynamic imaging experiments that promise to capture evolving processes in materials under operating conditions.

Big data and mathematical methods can build the bridge needed to link theory to experiment, Kalinin said. One problem has been data takes longer to process (e.g., a month on an 8-core computer) than acquire time (say, 10 hours). For ORNL's Borisevich, that problem had a solution. They acquired ultrafast data from STEM and piped it directly to the Titan supercomputer—which has 299,008 CPU cores to guide simulations while accompanying GPUs handle hundreds of calculations simultaneously—for analysis.

Experiment and theory work hand in hand to show how the real structure and function of a material compare to the ideal. Experiment helps inform and validate theory and theory-based models. “Highly resolved imaging techniques give information about atoms that need to be put into the theory. Then a model based on theory can tell properties. You can make inferences from that information,” according to ORNL theorist **Bobby Sumpter**. “Theory can connect pieces given from experiment, such as physics and mechanical properties and how they change upon for instance, introducing a dopant. You can fill in information and complete the story and move forward to ask, how can we make materials better?”

Whereas microscopy gives information about the surface of a material, neutron scattering digs deeper to give information about the bulk material. Combining the two can inform theories and models for predicting properties of designed materials, according to Sumpter. Kalinin said, “Once we have the infrastructure to stream our data from microscopes and we can measure structures and properties, we can start to build libraries of structure–property relationships on the single-defect level. We can verify libraries against X-ray and neutron scattering methods and know if a library is complete.”

Combining multimodal experiment and theory advances the advent of materials by design. “This is the first time in history we’ve matched experiment with theory,” Sumpter said. “We should have some success.” Success may mean understanding structural deviations called “defects” in atomically ordered materials. “Defects are not doom if you understand what they are and do,” Sumpter said.
ORNL’s **Thomas Proffen** works at SNS, which provides the world’s most intense pulsed neutron beams for scientific research and industrial development. This accelerator-based neutron source is next-door to CNMS and has approximately 20 beamline experiments that measure structures and dynamics of materials in diverse applications from biology to additive manufacturing. The data sets are huge. “Neutron data has a lifecycle from the time the neutron hits the detector to the identification of scientifically interesting data,” Proffen said. “When data sets are small, people can keep on top of it. Now we can’t.”

Proffen is the director of the neutron data analysis and visualization division in the Neutron Sciences Directorate of ORNL and also heads the Center for Accelerating Materials Modeling (CAMM), funded by BES specifically for direct integration of simulation and modeling into the analysis loop for data from neutron experiments. Direct integration allows scientists to refine theoretical models against experimental observations, use models to predict where new experimental measurements should be performed, and analyze some data at the user facility before taking it to the home institution for full analysis. “Neutron events are streamed and processed live, allowing a near-real-time view of collected data so a scientist running the experiment can make decisions on the fly,” Proffen said. “To visualize data, we play with everything from virtual reality headsets to volume rendering on parallelized servers.”

At Supercomputing 2014, ORNL researchers demonstrated the pipeline for diffuse scattering data of material defects. Through CAMM, researchers identify existing computational methods, such as pattern recognition and machine learning, providing new ways to extract data. If brute-force computing is to help process data from neutron scattering, Proffen said, future challenges include managing metadata (“data about data”), handling instrument and experiment configurations, and planning tools.

Scientists are producing so much data that the majority goes unanalyzed, according to **Thomas Potok,** who heads ORNL’s Computational Data Analytics group and led an automation project identifying research papers made possible through use of ORNL’s supercomputer to provide a metric of its scientific impact. Noting that data is published in papers that are the primary output of science, Kalinin asked Potok: Is there a better way to exploit papers to make additional discoveries? Potok set up automated tools that in part assigned greater weight to papers with higher impact factors and used them to find interesting papers, “in the Amazon sense of a ‘recommend’: ‘Hey! You bought this. Maybe you want this?' Look at some recommendations and you say, 'These people may be valuable to bring in to my next workshop.'"

The next step for text analytics is deep learning, which relies on computing. "The exciting thing is deep learning has made a lot of breakthroughs using GPUs," Potok said. "At Stanford they were able to recognize cat faces using a cluster of 64 GPUs. Well, we've got this Titan computer that's got 18,000 GPUs." National labs could deftly adopt off-the-shelf technologies to interpret imaging data in the form of text, including chemical and mathematical formulae, according to Kalinin.

During a meeting break, **Chad Steed** of ORNL entertained questions about data visualization, which processes data that is copious and complex. "We're combining computational analytics with interactive data visualization—the human part—so that we could bring in scientists' intuition and their background knowledge that you [might] lose with a purely data analytics approach," he said. A visual analytics system could essentially look over a scientist's shoulder and engage algorithms that learn from the scientist's interactions and improve its ability to predict what the scientist thinks is interesting. "It could build up a knowledge repository that a novice could use to start up with at least some of the initial capabilities of an expert scientist," Steed said. "Humans are very good at visual processing and intuition tasks that are hard to do with a computer. If we could grasp that strength of the humans in some type of intelligent interface, we could go after problems that neither approach in isolation could solve."

Discussing the path forward

The meeting concluded with a panel discussion, moderated by CNMS's **Christen**, of what DOE's nanoscience centers can and should do to help the scientific community strengthen the link between data and imaging sciences.

"We're transitioning from imaging being a qualitative tool to a quantitative tool," **Kalinin** pointed out. "This requires hardware platforms, and lo and behold because of the previous investment made by DOE and other funding agencies, these platforms exist. These platforms happen to be extremely data-intensive in terms of data generation and extremely demanding in terms of analytics. And at the same time we have all the capabilities enabled by supercomputing. This feels like a perfect storm."

To use knowledge from imaging to improve predictive theories, scientists need a proper mathematical framework implemented on machines they can use, **Kalinin** said.

Stach of Brookhaven's Center for Functional Nanomaterials said the lack of staff specifically associated with data management and data methods was a problem. "We don't have a central resource (for users and staff) where there's deep expertise in these areas," he said. Having on-board experts acting as liaisons to centers at the forefront of the big-data tsunami, such as light and neutron sources, could spur opportunities to gain knowledge of best practices and incorporate different approaches.

"We're still at the place where there's a lot of 'artisanal software' being put together," said **James Shuck,** director of Imaging and Manipulation of Nanostructures Facility at Berkeley's Molecular Foundry. "This is where we need people to start talking to one another. The data modeling people are starting to talk to the data generators; that's key. However, there's still plenty of jargon, which is a sign they're half talking past each other." The solution is having people who spend their time thinking about this. "This is an opportunity DOE and the NSRCs have. There's a reason the NSRCs are at the labs. It's because they are colocalized with other facilities. There's a chance for real interaction to occur."

Dean Miller of Argonne's Center for Nanoscale Materials agreed, emphasizing the need for standardized data formats**.** "We need teamwork," he said. "Vendors may have a proprietary format, but we can push them to make sure that their software will provide the data in an open-source data format as well."

Miller said his electron microscopy center is collocated with other facilities at the forefront of big-data management. "We're benefitting tremendously from [researchers at the collocated Advanced Photon Source] tackling many of these problems," he said. As the nation's nanocenters were built, community involvement and participation from other facilities were critical. "In terms of now addressing these challenges for data, that same strategy holds: We need community involvement to guide us."

"We absolutely need to be doing continuous education," **Kalinin of Oak Ridge's IFIM** said to an audience and panel enthusiastic about the suggestion. He cited the success of specialized "boot camp" workshops, e.g. in computing topics. "Those of us who got PhDs 10 years ago or more have very limited if any clue about the power of the modern statistical methods—computation and so on. As part of our regular job routine, the chances of doing it are remote," he said. "Without this, we simply won't be able to learn tools in the areas which are vital to us."

A university professor in the audience said, "I push my students, but they don't have the tools to use." She suggested students and teachers as well as scientists could benefit from boot-camp-style online teaching modules. Stach praised the National Science Foundation's nanoHUB tool to disseminate computer programs helpful in nanoscience and nanotechnology. "The effectiveness of online education is very clear," he said.

Shuck confessed awe at the fact that a colleague can take 3D tomographs, and while the experiment is ongoing, analyze and reconstruct the data in multiple ways and reask questions. "I couldn't do that three years ago. We've seen knowledge accelerate," he said. "If a tutorial is made, I'd like to take that class." He pointed out that many attendees of the DOE nanoscience-centers workshop were also planners of an data-related symposium at the upcoming meeting of the Materials Research Society and could suggest workshops or tutorials to benefit the broader community.

Original story by Dawn Levy:

- Shorter (workshop review): https://www.olcf.ornl.gov/wp-content/uploads/2012/07/ACSS_Final_v3.pdf
- Longer: http://www.doeleadershipcomputing.org/wp-content/uploads/2011/07/INCITE_IR_FINAL_7-19-11.pdf

CAPTION/CREDIT: The “Big, Deep and Smart Data Analytics in Materials Imaging” workshop included a welcome from ORNL’s Michelle Buchanan (top left), activities (top right) and poster sessions (bottom left) at which researchers could share findings as well as panel discussions (bottom right, with from left, Oak Ridge’s Hans Christen, Brookhaven’s Eric Stach, Berkeley’s James Shuck, Argonne’s Dean Miller, and Oak Ridge’s Sergei Kalinin.) Image credit: Oak Ridge National Laboratory, U.S. Dept. of Energy; photographer Genevieve Martin, photo collage Allison Gray

Workshop Recommendations

1. Integrated tool development: Based on the workshop, several common research topics were delineated, including

1. Mathematical tools for imaging, especially those based on compressed sensing (LBNL, ANL, PNNL) and Markov chain models (NIST, Purdue)
2. Ptychography (ANL and LBL for X-ray, LBL and ORNL for STEM)
3. Pipelines for direct data transfer from STEMs/XRay to HPC (LBL, BNL, ANL, etc)
4. Direct image quantification via atomic positions (ORNL, NCSU, NIST)

We note that the selection of these topics is driven by the physics of the imaging process (e.g., low dose imaging necessitates compressed sensing methods) or new opportunities for characterization of matter (ptychography, which effectively combines scattering and sub-atomic resolution imaging). Pursuing these directions in turn requires the development of the infrastructure (pipelines) and data analytics tools (visualization, unsupervised learning, reconstructions), in the absence of which the amount of information available for analysis is limited by human analysis and a selection bottleneck.

For these common topics, we recommend the integration of the software development effort across the NSRCs (and potentially beyond), including:

- Establishing common file format and systems for storing metadata
- Establishing universal code repository, e.g. based on GitHub
- Development of integrative platforms that allow cross-checking of the codes from different group and their availability for broad community via app-like system

The specific pathway to achieve this goal can be via informal meetings among PIs followed by the software development hackathons to establish the synergy in software development effort between the groups.

2. Cloud Imaging: The emergence of high-resolution aberration corrected imaging and ptychography in synergy with big data techniques signifies a paradigm shift of electron microscopy from *imaging* to *quantitative structural* tool much like synchrotrons and scattering facilities. Unlike the scattering facilities, this Big Data STEM infrastructure is likely to rely on distributed network of instrumental facilities and data analytics (imaging in the cloud). We believe that presently the field is posed on the brink of the fundamental paradigm change enabled by confluence of high-resolution imaging and full harnessing of information flow from the microscope, specifically by recording the complete scattering distribution at atomic resolution. The confluence of recent advances in instrumentation, detectors, and computing power will enable widespread adoption of ptychographic imaging as a universal STEM imaging mode, as a next paradigm beyond aberration-corrected imaging. Even though data generation rate for STEM in ptychographic mode can be comparable to that of the LHC, fully harnessing this data flow has the potential to revolutionize our capability to probe the structure and functionality of matter in 3D and with sub-atomic resolution. Among the benefits:

Lateral “super-resolution” - because images are not generated in the conventional manner, the usual resolution limits do not apply, allowing the extraction of structural information beyond existing barriers and potentially pushing information limit by an order of magnitude.

- Vertical super-resolution – just like in holography, the three-dimensional information is encoded in the dataset, which should allow characterization of all the atoms in a three-dimensional structure.
- Electrical and magnetic field data recovery without specialized probes or microscopes – approaches such as electron holography use sophisticated illumination schemes to partly recover the electron phase lost in integration on the detector. With a ptychographic data set, retrieving this information becomes a software, rather than a hardware, problem.

- Imaging physics – the goal is to extract as much information as possible from every electron. Phase determination will allow computational reconstruction of sample characteristics and refinement of the models of beam/matter interactions. Multiple detectors can be numerically applied, allowing all of the conventional images to be reconstructed from a single dataset. Unique numerical detector geometries optimized for specific properties that cannot be implemented in hardware can be applied this way.
- Combination with electron energy loss spectroscopy or other spectroscopy techniques holds as-yet unexplored potential.

To implement these aims, a targeted investment into better detector systems for the existing microscopes will be required across the board, including potential development of novel detection devices. This will result in massive increases in data volumes, which will in turn require advanced computing resources to store and to process the data. Pipelines from imaging instruments to advanced computing power, including development of software and mathematical tools, would have to be included. We envision a distributed infrastructure for data acquisition and analysis that would integrate imaging instruments and advanced computing resources. Such a system should ensure web-openness to other users and theorists, and comply with new regulatory requirements.

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Appendix A: Initial ad

NSRC Workshop "Big, deep, and smart data in materials imaging"

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June 8-10, 2015 at Oak Ridge National Laboratory, Oak Ridge, TN

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Point of contact: Amanda Zetans, **zetansac@ornl.gov**

Background: Understanding and ultimately designing improved functional materials that possess complex properties will require the ability to integrate and analyze data from multiple instruments designed to probe complementary ranges of space, time, and energy. Recent advances in imaging technologies have opened the floodgates of high-veracity information in the form of multidimensional data sets. These high-resolution images and spectra conceal unexamined information on atomic positions and local functionalities, as well as their evolution with time, temperature, and applied fields. To gain the full benefits of such data sets, we must be able to effectively interrogate them for a variety of physically and chemically relevant information, develop pathways for probing local structure-property relationships, and to synergistically link these results to atomistic theories (e.g., deep data analysis for scientific inference). The traditional simple graphical representation and visual inspection of such data sets are no longer sufficient to extract the most meaningful information. Advanced mathematical and computational methods are increasingly being incorporated into imaging sciences to deal with such "deep" data sets, and to combine data streams from different imaging techniques. However, many of the required mathematical or numerical tools are either lacking or not generally accessible to the imaging sciences community.

Scope: This workshop will bring together researchers from different imaging disciplines (electron microscopy, scanning probe microscopy, focused x-ray, neutron, atom probe tomography, chemical imaging, optical microscopies) as well as experts in mathematical/statistical/computational approaches to discuss opportunities and future needs in the integration of advanced data analytics and theory into imaging science. It will provide a forum to present achievements in the various imaging disciplines with emphasis on acquisition, visualization, and analysis of multidimensional data sets, the corresponding approaches for theory-experiment matching, and novel opportunities for instrumental development enabled by the availability of high speed data analytic tools.

Outcomes: The workshop aims to identify areas where advanced data analytics approaches will significantly increase the quality of information extracted from imaging data, and identify the role to be played by the NSRCs to make such approaches accessible to the user community. At the same time, the workshop will identify areas in which enhanced interaction with researchers in applied mathematics, statistics, theoretical and computational sciences will be most beneficial to the imaging and materials sciences community in particular, and nanosciences in general.

Format: The workshop will consist of plenary lectures to introduce the key areas of interest, contributed talks and posters, as well as panel discussions and breakout sessions to discuss the needs and opportunities in the various areas.

Tentative Topics include:

- Unsupervised learning for image analysis, classification, and information extraction
- Harnessing structural and functional imaging for materials development and discovery, for soft/hybrid as well as for hard materials
- Deep learning in imaging: Bayesian inference, parameter space compression, exploring unstructured data
- Integrating data sets from different imaging modalities and different length and time scales

Appendix B: Program

Joint NSRC Workshop – Big, Deep, and Smart Data Analytics in Materials Imaging

Program

(p): Plenary lecture, 45 min., including questions
(i): Invited talk, 30 min., including questions
(c): Contributed talk, 15 min., including questions
(d): Panel discussion, 30 min.

Monday, June 8:

7:30 – 8:15 Breakfast

8:15 – 8:30 Introduction (M. Buchanan, ORNL Associate Laboratory Director for Physical Sciences)
8:30 – 8:45 Introduction (J. Nichols, ORNL Associate Laboratory Director for Computational Sciences)
8:45 – 9:00 Introduction (H.M. Christen, Director, Center for Nanophase Materials Sciences)

9:00 – 10:30 Morning session 1

- T1 (p): J. Sethian (Berkeley), *CAMERA: The Center for Advanced Mathematics for Energy Research Applications*
- T2 (i): I. McNulty (ANL), TBD
- T3 (c): T. Potok (ORNL), *Beyond Gutenberg: A Computational Analysis Approach to Scientific Discovery and Innovation*

10:30 – 11:00 Coffee Break

11:00 – 12:30 Morning session 2

- T4 (i): E. Stach (BNL), *Creating a Big Data Ecosystem at the Brookhaven National Laboratory: Successes, challenges and needs*
- T5 (i): J. Ciston (NCEM, Berkeley), *Current Efforts and Future Needs for Recording, Visualizing and Analyzing Multidimensional Datasets in Transmission Electron Microscopy*
- T6 (i): D. Vine (ANL), *Real time phase retrieval in nanobeam ptychography*

12:30- 2:30 Lunch/poster session

2:30 – 4:00 Afternoon session 1

- T7 (i): P. Voyles (U. Wisc), *Extracting Materials Structure Knowledge from STEM Data*
- T8 (i): D. Ushizima (LBL), *Scaling Analytics for Image-based Experimental Data*
- (d) Panel session (B. MacCabe [Chair], J. Ciston, E. Stach, F. DeCarlo), *Big data infrastructure for Imaging – challenges and opportunities*

4:00 – 4:30 Coffee Break

4:30 – 5:45 Afternoon session 2

- T9 (i): Q. Chen (UIUC), *Insights from watching dynamics: from patchy spheres to anisotropic nanocrystals*
- T10 (c): B. Doughty (ORNL), *Reducing the Complexity of Ultrafast Transient Absorption Microscopy Data into Decay Associated Amplitude Maps*
- T11 (c): M. Drouhard (UTK), *Immersion Data Visualization using the Oculus Rift with Applications in Materials Science*
- T12 (c): M.A. Groeber (AFRL) - *DREAM.3D: Thoughts & Lessons Learned While Creating a Common Environment to Store, Share &Work With Digital Microstructure Data*

6:30 Dinner (by reservation only – Riverside Grill, 100 Melton Lake Peninsula, Oak Ridge, TN 37830)

Tuesday, June 9

7:30 – 8:30 Breakfast

8:30 – 10:30 Morning session 1

- T13 (i): S. Sankaranarayanan (ANL), *Imaging and visualizing ultrafast energy transport via molecular simulations*
- T14 (i): D. Skinner (LBL), *Design Patterns in Web-based HPC : Materials Imaging*
- T15 (i): T. Proffen (ORNL), *Neutrons, Materials and Data Challenges*
- (d) Panel session (B. Sumpter [Chair], S. Sankaranarayanan, D. Skinner, P. Kotula) *Linking big data to computing for materials design*

10:30 – 11:00 Coffee

11:00 – 12:30 Morning session 2

- T16 (i): K. Kleese van Dam (PNNL), *Towards streaming analysis of dynamic imaging experiments*
- T17 (c): E. Lagerfeld (ORNL), *A New Computational Infrastructure for the Advanced Analysis of Nanophase Materials Imaging*
- T18 (c): W.C. Yang (NIST), *Automatic Image Analysis of High Resolution Videos Obtained Using Environmental Transmission Electron Microscopy*

- T19 (i): N. Browning (PNNL), *Using Compressive Sensing, Statistics and Automated Tracking Algorithms to Optimize Data Acquisition in High-Resolution In-Situ TEM experiments*

12:30- 2:30 Lunch/poster session

2:30 – 3:45 Afternoon session 1

- T20 (i): M.J. Demkowicz (MIT), *Bringing Bayesian methods into the materials modeling mainstream*
- T21 (c): Rick Archibald (ORNL), *Sparse sampling methods for image processing and data analysis*
- T22 (c): M. Comer (Purdue), *Stochastic Modeling for Materials Images*
- T23 (c): R. Patton (ORNL), *Large-Scale Deep Learning for Scientific Discovery*

3:45 – 4:15 Coffee

4:15 – 5:45 Afternoon session 2

- T24 (i): A. Borisevich (ORNL), *Discovering Materials Physics in Real Space by STEM*
  T25 (i): J. LeBeau (NCSU), *Quantifying the whole STEM image: where we are and where to go from here*
- (d) Panel session (M. Demkowicz [Chair], S. Kalinin, K. Kleese van Dam, J. LeBeau) *Inverse problems and Bayesian inference in image analysis*

6:30 Dinner (on your own)

Wednesday, June 10:

7:30 – 8:30 Breakfast
8:30 –10:30 Morning session 1

- T26 (i): A. Lupini (ORNL), *Electron Ptychography in STEM*
- T27 (c): S. Patala (NCSU), *Identification of Atomic Clusters through Point-Pattern Matching Algorithms*
- T28 (c): D. Frank Ogletree (Berkeley), *Smart Imaging With Scanned Electrons*
- T29 (i): P. Kotula (Sandia), *Acquisition, Analysis and Quantification of Hyperspectral Images*
- T30 (i): D. Gursoy (ANL), *Compressive sampling and its potentials in nanoimaging*

10:30 – 11:00 Coffee

11:00 – 12:30 Morning session 2

- T31 (i): F. DeCarlo (Argonne), *Data intensive science at synchrotron based 3D X-ray imaging facilities: the Argonne National Laboratory experience from data-limited to data-intensive to data-driven science*
- T32 (c): L. Drummy (AFRL), *Data Analytics in Materials Characterization at AFRL*
- T33 (c): S.V. Kalinin (ORNL), *Big data in SPM*

- (d) Panel session (H. Christen [Chair], E. Stach, D. Miller, J. Schuck, S. Kalinin) *Role of NSRCs in integration of big data and imaging: science and user programs*

Appendix C: List of attendees

Rick Archibald
ORNL
US Government/Government Contractor
Bethel Valley Rd
Oak Ridge TN 37831
Work: 865-456-1405
E-Mail: archibaldrk@ornl.gov

Arthur Baddorf
Oak Ridge National Laboratory
US Government/Government Contractor
1 Bethel Valley Road
PO Box 2008, MS 6487
OAK RIDGE TN 37831
Work: 865-574-5241
E-Mail: baddorfap@ornl.gov

Feng Bao
Oak Ridge National Laboratory
US Government/Government Contractor
One Bethal Valley Road
Oak Ridge TN 37831
Work: 865-576-4325
E-Mail: baof@ornl.gov

Edward Barnard
Molecular Foundry
US Government/Government Contractor
Lawrence Berkeley National Lab
BERKELEY CA 94708
Work: 6507969301
E-Mail: esbarnard@lbl.gov

Richard Barnard
Oak Ridge National Laboratory
US Government/Government Contractor
1 Bethel Valley Rd
Bldg 5700
OAK RIDGE TN 37831
Work: 8653096962
E-Mail: barnardrc@ornl.gov

Alex Belianinov
CNMS ORNL
US Government/Government Contractor
1 Bethel Valley Rd
OAK RIDGE TN 37830
Work: 8652413083
E-Mail: ba8@ornl.gov

Tom Berlijn
Oak Ridge National Laboratory
US Government/Government Contractor
1 Bethel Valley Road
Oak Ridge TENNESSEE 37830
Work: 6313563062
E-Mail: tberlijn@gmail.com

Jean Bilheux
Oak Ridge National Laboratory - SNS
US Government/Government Contractor
1 Bethel Valley Road - MS 3475
Oak Ridge TN 37830
Work: 8654061704
E-Mail: bilheuxjm@ornl.gov

Dan Bocek
Asylum Research, Oxford Instruments
Private Industry/Other
6310 Hollister Avenue
SANTA BARBARA CA 93117
Work: 8056966466
E-Mail: dan.bocek@oxinst.com

Albina Borisevich
Oak Ridge National Laboratory
US Government/Government Contractor
1 Bethel Valley Rd
OAK RIDGE TN 37831
Work: 865-576-4060
E-Mail: albinab@ornl.gov

Nigel Browning
Pacific Northwest National Laboratory
US Government/Government Contractor
902 Battelle Boulevard
PO Box 999, MS: K2-12
RICHLAND WA 99352
Work: 509-375-7569
Fax: 509-371-6498
E-Mail: nigel.browning@pnnl.gov

Jihua Chen
CNMS
US Government/Government Contractor
One Bethel Valley Rd
Oak Ridge TN 37831
Work: 8655763385
E-Mail: chenj1@ornl.gov

Hans Christen
Oak Ridge National Laboratory
US Government/Government Contractor
PO Box 2008
Oak Ridge TN 37831
Work: 8655745081
E-Mail: christenhm@ornl.gov

Jim Ciston
Lawrence Berkeley National Laboratory
US Government/Government Contractor
Molecular Foundry One
Cyclotron Road
BERKELEY CA 94720
Work: 5104958072
E-Mail: jciston@lbl.gov

Mary Comer
Purdue University
US Student/Faculty
465 Northwestern Ave
WEST LAFAYETTE IN 47907
Work: 765-661-5815
E-Mail: comerm@purdue.edu

Valentino Cooper
Oak Ridge National Laboratory
US Government/Government Contractor
1 Bethel Valley Rd
OAK RIDGE TN 37830
Work: 865-483-8616
E-Mail: coopervr@ornl.gov

Cory Czarnik
Gatan
Private Industry/Other
5794 W. Las Positas Blvd
PLEASANTON CA 94588
Work: 4084727468
E-Mail: cczarnik@gatan.com

Eduardo D'Azevedo
Computer Science and Mathematics Division US Government/Government Contractor Oak Ridge National Laboratory
Bldg 5700, MS 6164
OAK RIDGE TN 37831
Work: 8655767925
E-Mail: dazevedoef@ornl.gov

Francesco De Carlo
Argonne National Laboratory
US Government/Government Contractor
9700 S. Cass Avenue
ARGONNE IL 60439
Work: 6302520148
E-Mail: decarlo@anl.gov

Francesco De Carlo
Argonne National Laboratory
US Government/Government Contractor
9700 S. Cass Av.
ARGONNE IL 60439
Work: 6302520148

E-Mail: decarlo@aps.anl.gov

Michal Demkowicz
MIT
US Student/Faculty
77 Massachusetts Ave.
CAMBRIDGE MA 02139
Work: 617-324-6563

E-Mail: demkowicz@mit.edu

Dane deQuilettes
University of Washington
US Student/Faculty
36 Bagley Hall
SEATTLE WA 98195
Work: 5092930211

E-Mail: dwd2@uw.edu

Peter Doak
UT Battelle
US Government/Government Contractor
Oak Ridge National Laboratory
PO BOX 2008 MS6493
OAK RIDGE TN 37831
Work: 865-407-3995

E-Mail: doakpw@ornl.gov

Benjamin Doughty
Oak Ridge National Laboratory
US Government/Government Contractor
1 Bethel Valley Road
4100 A155
OAK RIDGE TENNESSEE 37831
Work: 8655748955

E-Mail: doughtybl@ornl.gov

Margaret Drouhard
Department of EECS
US Student/Faculty
University of Tennessee
1520 Middle Drive
KNOXVILLE TN 37996
Work: 865-630-0634
E-Mail: meg.drouhard@utk.edu

Larry Drummy
Air Force Research Laboratory
US Government/Government Contractor
2941 Hobson Way
AFRL/RXAS
Wright Patterson AFB OH 45433
Work: 9372559160

E-Mail: lawrence.drummy.1@us.af.mil

Joseph Dycus
North Carolina State University
Select One
3603 Helix Court
Apt 201
RALEIGH NORTH CAROLINA 27606
Work: 8657762674
E-Mail: jhdycus@ncsu.edu

Jacob Eapen
North Carolina State University
US Student/Faculty
Department of Nuclear Engineering

2500 Stinson Drive
RALEIGH NORTH CAROLINA 27695
Work: 9195155952
E-Mail: jeapen@ncsu.edu

Barbara Evans
Oak Ridge National Laboratory
US Government/Government Contractor
P. O. Box 2008

4100 MS 6106
OAK RIDGE TN 37831
Work: 1-(865)-241-3185
E-Mail: evansb@ornl.gov

Erik Ferragut
Oak Ridge National Laboratory
US Government/Government Contractor
1 Bethel Valley Rd

OAK RIDGE TN 37831
Work: 865-230-2933
E-Mail: efn@ornl.gov

Emre Firlar
Ames Laboratory
US Government/Government Contractor
216A Wilhelm Hall
Iowa State University
AMES IA 50011
Work: 5516975639
E-Mail: efirlar@ameslab.gov

Michael Fitzsimmons
Oak Ridge National Lab
US Government/Government Contractor
PO Box 2008 MS 6475
OAK RIDGE TN 37932
Work: 5059010534

E-Mail: fitzsimmonsm@ornl.gov

Miguel Fuentes-Cabrera
Center for Nanophase Materials Sciences, ORNL
US Government/Government Contractor
1 Bethel Valley Road
OAK RIDGE TN 37831
Work: 865-574-2206

E-Mail: fuentescabma@ornl.gov

Zheng Gai
Oak Ridge National Lab
US Government/Government Contractor
43 Palisades PKWY
OAK RIDGE TENNESSEE 37830
Work: 8652749039

E-Mail: zgai@yahoo.com

Panchapakesan Ganesh
Oak Ridge National Laboratory
US Government/Government Contractor
1 Bethel Valley Rd.
PO BOX 2008 MS6494
OAK RIDGE TN 37831
Work: 8655741999

E-Mail: ganeshp@ornl.gov

Anthony Gianfrancesco
University of Tennessee Knoxville
US Student/Faculty
790 North Cedar Bluff Rd
Apt 2108
KNOXVILLE TENNESSEE 37923
Work: 4013166670

E-Mail: plasmant@gmail.com

Garrett Granroth
Neutron Data Analysis and Visualization Division
US Government/Government Contractor
PO BOX 2008 MS6475
OAK RIDGE TN 37831
Work: 865-805-0631
E-Mail: granrothge@ornl.gov

Adrienne Greene
Sandia National Labs
US Government/Government Contractor
PO Box 5800
MS1314
ABQ NM 87185
Work: 505-844-7482
E-Mail: acgreen@sandia.gov

Michael Groeber
Air Force Research Laboratory
US Government/Government Contractor
2230 Tenth St. Building 655 Room 079
WPAFB OH 45433
Work: 937-255-1317
E-Mail: michael.groeber@us.af.mil

Doga Gursoy
Argonne National Laboratory
US Government/Government Contractor
9700 South Cass Ave. 438-B003
LEMONT IL 60439
Work: 630-252-088
E-Mail: dgursoy@aps.anl.gov

Mark Hagmann
NewPath Research L.L.C.
Private Industry/Other
2880 S. Main Street, Suite 214
SALT LAKE CITY UTAH 84115
Work: 801-573-9853
E-Mail: mhagmann@newpathresearch.com

Steven Hahn
Oak Ridge National Laboratory
US Government/Government Contractor
Oak Ridge National Laboratory
PO Box 2008 MS6454
OAK RIDGE TENNESSEE 37831
Work: 5155201934
E-Mail: hahnse@ornl.gov

Jeffrey Harrison
University of Washington
US Student/Faculty
5027 9th AVE NE
Apt. A
SEATTLE WA 98105
Work: 4259228414
E-Mail: jarrisonwins@gmail.com

Todd Hastings University of Kentucky
US Student/Faculty
Electrical and Computer Engineering
453 F Paul Anderson Tower
Lexington KY 40506
Work: 859-218-6544
E-Mail: todd.hastings@uky.edu

Qian He
ORNL
US Government/Government Contractor
1 Bethel Valley Rd
Oak Ridge TENNESSEE 37830
Work: 4847672898
E-Mail: heq1@ornl.gov

Thomas Henage
NewPath Research L.L.C.
Private Industry/Other
2880 S. Main Street, Suite 214
SALT LAKE CITY UTAH 84115
Work: 801-573-9853
E-Mail: thenage@gmail.com

Dale Hensley
CNMS
US Government/Government Contractor
One Bethel Valley Road
OAK RIDGE TN 37831
Work: 865-576-6697
Fax: 865-574-1753
E-Mail: hensleydk@ornl.gov

Hoi-Ying Holman
Lawrence Berkeley National Laboratory
US Government/Government Contractor
MS 70A-3317
One Cyclotron Road
Berkeley CA 94720
Work: 5105865943
E-Mail: hyholman@lbl.gov

Holland Hysmith
Oak Ridge Nationaly Laboratory
US Government/Government Contractor
1 Bethel Valley Rd
OAK RIDGE TN 38731
Work: 865-574-4871
E-Mail: holland.hysmith@gmail.com

Vighter Iberi
Center for Nanophase Materials Sciences
US Student/Faculty
Oak Ridge National Laboratory
1 Bethel Valley Road
Oak Ridge TENNESSEE 37831
Work: 865-438-9500
E-Mail: iberivo@ornl.gov

Anton Ievlev
Oak Ridge National Laboratory
US Government/Government Contractor
1 Bethel valley rd
Oak Ridge TN 37831
Work: 8652428658
E-Mail: ievlevav@ornl.gov

Russell Jacobs
Self
Private Industry/Other
PO Box 1456
PEMBROKE NC 28372
Work: 910-785-3027
E-Mail: rjacobs@yahoo.com

Yuanwen Jiang
the University of Chicago
US Student/Faculty
929 E 57th St. GCIS ESB 021
CHICAGO IL 60637
Work: 3128880910
E-Mail: yuanwen@uchicago.edu

Yang Jiao
Arizona State University
US Student/Faculty
ERC 387
PO BOX 876106
TEMPE ARIZONA 85287-6106
Work: 4809654560
E-Mail: yang.jiao.2@asu.edu

Wayne Joubert
Oak Ridge National Laboratory
US Government/Government Contractor
1 Bethel Valley Road, MS-6008
Oak Ridge TN 37831
Work: 8652412835
E-Mail: joubert@ornl.gov

Sergei Kalinin
ORNL
US Government/Government Contractor
1 Bethel Valley Rd. OAK
RIDGE TN 37831
Work: (865)2410246
E-Mail: sergei2@ornl.gov

Durmus Karatay
University of Washington
US Student/Faculty University
of Washington MoES Building
Room G44B Seattle
WASHINGTON 98195
Work: 2062214191
E-Mail: ukaratay@uw.edu

Kerstin Kleese van Dam
Pacific Northwest National Laboratory
US Government/Government Contractor
902 Batelle Boulevard
RICHLAND WA 99352
Work: 5093717797
E-Mail: kerstin.kleesevandam@pnll.gov

Paul Kotula
Sandia National Laboratories
US Government/Government Contractor
PO Box 5800, MS 0886
ALBUQUERQUE NM 87185-0886
Work: 505-844-8947
E-Mail: pgkotul@sandia.gov

Ivan Kravchenko
ORNL
US Government/Government Contractor
One Bethel Valley Road
P.O.Box 2008, MS-6487
Oak Ridge TN 37831
Work: 865-576-6457
E-Mail: kravchenkoii@ornl.gov

Mikhail Kravchenko
University of Tenessee Knoxville
US Student/Faculty
4503 christine lynnac st
KNOXVILLE TN 37938
Work: 352-281-1960
E-Mail: mkravche@vols.utk.edu

A. Gilad Kusne
NIST
US Government/Government Contractor
100 Bureau Dr
GAITHERSBURG MD 20899
Work: 4129151433
E-Mail: aaron.kusne@nist.gov

Nouamane Laanait
CNMS / Oak Ridge National Lab
US Government/Government Contractor
P.O. Box 2008
oak Ridge TN 37831
Work: 8655742988
E-Mail: laanaitn@ornl.gov

James LeBeau
North Carolina State University
US Student/Faculty
911 Partners Way
RALEIGH NC 27606
Work: 919-515-5049
E-Mail: jmlebeau@ncsu.edu

Steven Lee
U.S. Department of Energy
US Government/Government Contractor
1000 Independence Avenue, S.W. SC-
21, Germantown Building
WASHINGTON DC 20585-1290
Work: 301-903-5710
E-Mail: steven.lee@science.doe.gov

Hechao Li
Arizona State University
US Student/Faculty
ERC 387
PO BOX 876106
TEMPE ARIZONA 85287-6106
Work: 4809654560
E-Mail: hechaoli@asu.edu

Lianshan Lin
Oak Ridge National Laboratory
US Government/Government Contractor
OAK RIDGE NATIONAL
LABORATORY PO BOX 2008 MS6069
OAK RIDGE TN 37831
Work: 8652414531
E-Mail: linl@ornl.gov

Eric Lingerfelt
Oak Ridge National Laboratory
US Government/Government Contractor
One Bethel Valley Road
P.O. Box 2008
Oak Ridge TN 37831
Work: 8655766618
E-Mail: lingerfeltej@ornl.gov

Arthur Maccabe
Oak Ridge National Laboratory
US Government/Government Contractor
PO Box 2008
Oak Ridge TN 37831
Work: 865-241-6504
Fax: 865-574-6076
E-Mail: maccabeab@ornl.gov

Artem Maksov
UT/ORNL Bredesen Center
US Student/Faculty
5700 Pleasant Ridge Rd
Apt. #515
KNOXVILLE TN 37912
Work: 413-3558276
E-Mail: maksovab@ornl.gov

Jason Maldonis
University of Madison, Wisconsin
US Student/Faculty
1509 University Ave
Madison WISCONSIN 53706
Work: 6082955532
E-Mail: maldonis@wisc.edu

George Maracas
DOE Office of Science
US Government/Government Contractor
1000 Independence Ave, SW
SC 22.3, Germantown Bldg., F-429A
Washington DC 205851290
Work: 301903164
E-Mail: george.maracas@science.doe.gov

Baishakhi Mazumder
Oak Ridge National LAboratory
US Government/Government Contractor
1 Bethal valley road
OAK RIDGE TENNESSEE 37830
Work: 8655766994
E-Mail: mazumderb@ornl.gov

Kristin McCullough
Grand View University
US Student/Faculty
1200 Grandview Ave
DES MOINES IOWA 50316
Work: 8152808928
E-Mail: kmccullo4@gmail.com

Ian McNulty
Argonne National Laboratory
US Government/Government Contractor
Bldg. 440, Room A-140
9700 S. Cass Ave.
ARGONNE IL 60439
Work: 630-252-2882
E-Mail: mcnulty@anl.gov

Stephen Mick
Gatan
Private Industry/Other
1762 CR 213
Weimar TX 78962
Work: 9199464399
E-Mail: smick@gatan.com

Dean Miller
Argonne National Laboratory
Select One
9500 S Cass Ave
ARGONNE ILLINOIS 60439
Work: 6302524108
E-Mail: miller@anl.gov

Rohan Mishra
Vanderbilt University
US Student/Faculty
1 Bethel Valley Rd
OAK RIDGE TENNESSEE 37830
Work: 6142642450
E-Mail: rohan.mishra@vanderbilt.edu

Eva Mutunga
Bredesen Center at University of Tennessee, Knoxville
Non-US Student/Faculty
1700 W. Clinch Ave
Apt 419
KNOXVILLE TN 37916
Work: 301-646-9976
E-Mail: Emutunga@vols.utk.edu

Hugh O'Neill
Oak Ridge National Laboratory
US Government/Government Contractor
PO Box 2008
OAK RIDGE TN 37831
Work: 865 574 5283
E-Mail: oneillhm@ornl.gov

D Frank Ogletree
Lawrence Berkeley National Lab
US Government/Government Contractor
Molecular Foundry
MS 67R2206
BERKELEY CA 94720
Work: 510 486 4862
E-Mail: dfogletree@lbl.gov

M. Baris Okatan
ORNL CNMS
US Government/Government Contractor
ORNL CNMS
Oak Ridge TN 37831
Work: 8659641040
E-Mail: m.b.okatan@gmail.com

Colin Ophus
Lawrence Berkeley National Laboratory
US Student/Faculty
1 Cyclotron Road
Berkeley CA 94720
Work: 510-486-5663
E-Mail: clophus@lbl.gov

Johanna Palmstrom
Stanford University
US Student/Faculty
25 Olmsted Road Apt 105
STANFORD CA 94305
Work: 9523537010
E-Mail: jpalms@stanford.edu

Jewook Park
Oak Ridge National Laboratory
US Government/Government Contractor
One Bethel Valley Road P.O.Box 2008
OAK RIDGE TN 37831-6487
Work: (865)574-9393
E-Mail: parkj1@ornl.gov

Srikanth Patala
North Carolina State University
US Student/Faculty
911 partners way
RALEIGH NORTH CAROLINA 27695
Work: 9195153039
E-Mail: spatala@ncsu.edu

Robert Patton
Oak Ridge National Laboratory
US Government/Government Contractor
PO Box 2008
MS-6085
OAK RIDGE TN 37831
Work: 8655763832
E-Mail: pattonrm@ornl.gov

Thomas Potok
Oak Ridge National Lab
US Government/Government Contractor
1 Bethel Valley Road
Oak Ridge TN 37831
Work: 865-574-0834
E-Mail: potokte@ornl.gov

Dhiren Pradhan University of Puerto Rico US Student/Faculty
Department of Physics
University of Puerto Rico,P.O. BOX 70377
SAN JUAN PR - PUERTO RICO 00936-8377
Work: 7874132208
Fax: 7877642571
E-Mail: dhirenkumarp@gmail.com

Thomas Proffen
Oak Ridge National Laboratory
US Government/Government Contractor
Neutron Science
PO. Box 2008, MS 6475
OAK RIDGE TN 37831-6475
Work: 8655768633
Fax: 8655746080
E-Mail: tproffen@ornl.gov

Tanya Prozorov
Ames Lab Select
One
Division of Materials Sciences and Engineering
332 Wilhelm Hall
AMES IOWA 50011
Work: 5152943376
E-Mail: tprozoro@ameslab.gov

Weiju Ren
Oak Ridge National Laboratory
US Government/Government Contractor
1 Bethel Valley Road
Room 239, Building 4515
OAK RIDGE TN 37831-6069
Work: 865-576-6402
E-Mail: renw@ornl.gov

Robert Sacci
ORNL
US Government/Government Contractor
1 Bethel Valley Rd
OAK RIDGE TN 37831
Work: 8652415135
E-Mail: saccirl@ornl.gov

Ritesh Sachan
Oak Ridge National Laboratory
US Government/Government Contractor
PO Box 2008, MS6071
Oak Ridge National Laborratory
Oak Ridge TENNESSEE 37831
Work: 865-293-9248
E-Mail: sachanr@ornl.gov

Jerzy Sadowski
Brookhaven National Laboratory
US Government/Government Contractor
Center for Functional Nanomaterials
Bldg. 735
UPTON NY 11973
Work: (631) 344-8077
E-Mail: sadowski@bnl.gov

Subramanain Sankaranarayanan
Argonne National Laboratory
US Government/Government Contractor
9700 S Cass Avenue
Argonne IL 60439
Work: 6302524941
E-Mail: skrssank@anl.gov

Subramanain Sankaranarayanan
Argonne National Laboratory
US Government/Government Contractor
9700 S Cass Avenue
Argonne IL 60439
Work: 6302524941
E-Mail: skrssank@anl.gov

P James Schuck
The Molecular Foundry, LBNL
US Government/Government Contractor
1 Cyclotron Road
BERKELEY CA 94720
Work: 650-279-6530
E-Mail: pjschuck@lbl.gov

Pablo Seleson
Oak Ridge National Laboratory
US Government/Government Contractor
One Bethel Valley Road
P.O. Box 2008, MS 6164
OAK RIDGE TN 37831
Work: (865) 576-2859
E-Mail: selesonpd@ornl.gov

Fatih Sen
Argonne National Laboratory
US Government/Government Contractor
Center for Nanoscale Materials
9700 S Cass Ave
LEMONT IL 60439
Work: 630-252-7789
E-Mail: fsen@anl.gov

Jeff Simmons
Air Force Research Laboatory
US Government/Government Contractor
2230 Tenth St
Wright-Patterson AFB, Area B
WRIGHT-PATTERSON OH 45433
Work: 9372551346
E-Mail: jeff.simmons.3@us.af.mil

Mary Jane Simpson
Oak Ridge National Lab
US Government/Government Contractor
PO BOX 2008 MS6142
OAK RIDGE TN 37831-6142
Work: 3212778417
E-Mail: simpsonm@ornl.gov

David Skinner
Lawrence Berkeley National Lab
US Government/Government Contractor
1 Cyclotron Road
BERKELEY CA 94706
Work: 510-486-4748
E-Mail: deskinner@lbl.gov

Patrick Smith
University of Texas/ austin
US Student/Faculty
400 B Buena Vista
WESTLAKE HILLS TX 78746
Work: 5124758786
E-Mail: patrick.smith@beg.utexas.edu

Suhas Sreehari
Purdue University
US Student/Faculty
2550 Yeager Road
Apt. 13-5
West Lafayette IN 47906
Work: 6468120677
E-Mail: ssreehar@purdue.edu

Eric Stach
Brookhaven National Laboratory
US Government/Government Contractor
Center for Functional Nanomaterials
UPTON NY 11733
Work: 765-346-3460
E-Mail: estach@bnl.gov

Chad Steed
Oak Ridge National Laboratory
US Government/Government Contractor
1 Bethel Valley Rd. OAK
RIDGE TN 37831
Work: 8655747168
E-Mail: steedca@ornl.gov

Andrew Stevens
Duke University
US Student/Faculty
3029 Bluffs Dr
RICHLAND WASHINGTON 99354
Work: 5094325997
E-Mail: ajs104@duke.edu

Joshua Stuckner
Virginia Tech
US Student/Faculty
400 Fairfax Rd
Apt M99
BLACKSBURG VA 24060
Work: 5402195221
E-Mail: stuckner@vt.edu

Bobby Sumpter
Oak Ridge National Laboratory
US Government/Government Contractor
Center for Nanophase Materials Sciences
Oak Ridge TENNESSEE 37831-6494
Work: 865-574-
E-Mail: sumpterbg@ornl.gov

Christopher Symons
Oak Ridge National Laboratory
US Government/Government Contractor
1 Bethel Valley Road
Oak Ridge TENNESSEE 37831
Work: 865-241-5952
E-Mail: symonsct@ornl.gov

Bryan Thompson
SYSTAP, LLC
Private Industry/Other
4501 Tower Road
GREENSBORO NC 27410
Work: 2024629888
E-Mail: bryan@systap.com

Ho Ming Tong
University of Florida/ Chemical Engineering
US Student/Faculty
2330 Woodbine Ave
KNOXVILLE TN 37917
Work: 6787707956
E-Mail: gabriel.tong@ufl.edu

Raymond Unocic
Center for Nanophase Materials Science
US Government/Government Contractor
Oak Ridge National Laboratory
One Bethel Valley Road
OAK RIDGE TN 37831
Work: 865-574-0096
E-Mail: unocicrr@ornl.gov

Daniela Ushizima
LBNL
US Government/Government Contractor
1 cyclotron
BERKELEY CA 94720
Work: 4157100587
E-Mail: dushizima@lbl.gov

Rama Vasudevan
OAK RIDGE NATIONAL LABORATORY
US Government/Government Contractor
1 BETHEL VALLEY RD
OAK RIDGE TN 37831
Work: 18652414174
E-Mail: rvv@ornl.gov

Ranga Vatsavai
North Carolina State University
US Student/Faculty
332 Terrastone Pl
Cary NORTH CAROLINA 27519
Work: 8652476355
E-Mail: rrvatsav@ncsu.edu

Mario Viani
Asylum Research, Oxford Instruments
Private Industry/Other
6310 Hollister Avenue
SANTA BARBARA CA 93117
Work: 8056966466
E-Mail: mario.viani@oxinst.com

David Vine
Argonne National Lab
US Government/Government Contractor
9700 S Cass Ave
ARGONNE IL 60439
Work: 6302521984
E-Mail: dvine@anl.gov

Sarah Vorpahl
University of Washington Seattle
US Student/Faculty
Department of Chemistry, University of Washington
Box 351700
Seattle WA 98195
Work: 6107511714
E-Mail: svorpahl@uw.edu

Paul Voyles
University of Wisconsin-Madison
US Student/Faculty
1509 University Ave
MADISON WI 53706
Work: 608-772-9726
E-Mail: paul.voyles@wisc.edu

Song Wang
University of South Carolina
US Student/Faculty
Department of Computer Science and Engineering
University of South Carolina
COLUMBIA SOUTH CAROLINA 29208
Work: 8038007932
E-Mail: songwang@cec.sc.edu

Jack Wells
Oak Ridge National Laboratory
US Government/Government Contractor
PO Box 2008
MS 6008
Oak Ridge TN 37831-6008
Work: 865-660-2758
E-Mail: wellsjc@ornl.gov

Jim Werner
Los Alamos National Laboratory
US Government/Government Contractor
Center for Integrated Nanotechnologies
LOS ALAMOS NM 87545
Work: 505-667-8842
E-Mail: jwerner@lanl.gov

Tracy Whitaker
Oak Ridge National Laboratory
US Government/Government Contractor
1 Bethel Valley Road
OAK RIDGE TN 37831-6488
Work: 865-241-8268
E-Mail: whitakerth@ornl.gov

Kai Xiao
Oak Ridge National Laboratory
US Government/Government Contractor
One bethel valley road
OAK RIDGE TN 37831
Work: 8655747690
E-Mail: xiaok@ornl.gov

Kyle Yakal-Kremski
National Academy of Sciences
US Government/Government Contractor
500 5th St NW
WASHINGTON DC 20001
Work: 2016023931
E-Mail: kyle.yakal-kremski.ctr@nrl.navy.mil

Sangmo Yang
CNMS/ORNL
US Government/Government Contractor
1 Bethel Valley Road, Bldg. 8610, MS 6487, P. O. Box 2008
Oak Ridge TN 37831
Work: 865-607-5005
E-Mail: yangs@ornl.gov

Wei-Chang Yang
Center for Nanoscale Science and Technology US Government/Government Contractor National Institute of Standards & Technology
100 Bureau Dr. Mail Stop 6203
GAITHERSBURG MD 20899
Work: 301-975-8398
E-Mail: david.yang@nist.gov

Hongkai Yu
University of South Carolina
US Student/Faculty
315 Main St.
Computer Science and Engineering Dept.
COLUMBIA SC 29208
Work: 4358904634
E-Mail: yu55@email.sc.edu

Dmitri Zakharov
Center for Functional Nanomaterials
US Government/Government Contractor
Brookhaven National Laboratory
PO Box 5000
Upton NY 11973
Work: 631-344-3507
E-Mail: dzakharov@bnl.gov

Amanda Zetans
CNMS
US Government/Government Contractor
1 Bethel Valley Road
OAK RIDGE TN 37830
Work: 865-241-1182
E-Mail: zetansac@ornl.gov

Jiaming Zhang
Hewlett Packard Labs
Private Industry/Other
1501 Page Mill Rd
Palo Alto CALIFORNIA 94304
Work: 6506901395
E-Mail: jiamingzhang98@gmail.com

Minghao Zhang
UCSD
US Student/Faculty
9450 Gilman Dr., UCSD #40090
LA JOLLA CALIFORNIA 92092
Work: 8589569058
E-Mail: miz016@eng.ucsd.edu

Wu Zhou
Oak Ridge National Laboratory
US Government/Government Contractor
1 Bethel Valley Rd
Oak Ridge TN 37831
Work: 8655748899
E-Mail: zhouw1@ornl.gov

Youjie Zhou
University of South Carolina
US Student/Faculty
315 Main St.
Computer Science and Engineering Dept.
COLUMBIA SC 29208
Work: 3025884856
E-Mail: zhou42@email.sc.edu