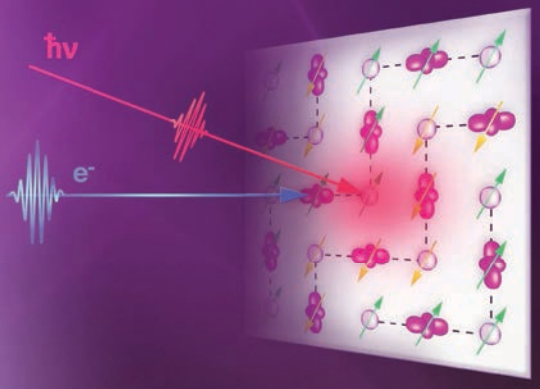
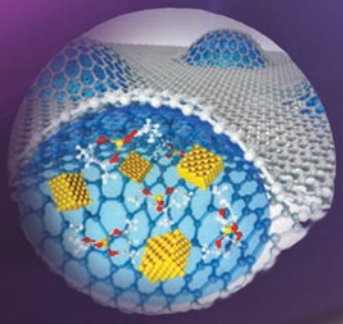
FUTURE OF ELECTRON SCATTERING & DIFFRACTION

Report of the Basic Energy Sciences Workshop
on the Future of Electron Scattering and Diffraction
February 25-26, 2014





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Front cover

From top right to bottom left: 1) Schematic of electron-beam based ultrafast experiment using photons as an excitation source to understand charge, orbital and lattice correlation; 2) Atomic image of SiN obtained via electron exit-wave reconstruction using the TEAM-0.5 double-aberration-corrected scanning transmission electron microscope (STEM) at NCEM. Distance between the neighboring atoms of the hexagonal cell is 0.18nm; 3) Position averaged convergent beam electron diffraction pattern acquired in STEM that allows for unit-cell-by-unit-cell symmetry mapping of correlated oxides; and 4) Schematic of nano encapsule enabling observation of dynamic materials processes at the atomic level in situ and operando.

Report of the Basic Energy Sciences Workshop on Future of Electron Scattering and Diffraction

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Abbreviations

3D	Three Dimensional
Å	Angstrom
APT	Atom Probe Tomography
BES	Basic Energy Sciences
DDD	Direct Electron Detector
DQE	Detector Quantum Efficiency
EBIC	Electron Beam Induced Current
EDS	Energy-Dispersive X-ray spectroscopy
EELS	Electron Energy Loss Spectroscopy
ETEM	Environmental Transmission Electron Microscope
FEL	Free Electron Laser
fs	Femtosecond
HAADF	High-Angle Annular Dark-Field
MOFs	Metal-Organic Frameworks
IR	Infrared
MEMS	Micro-Electro-Mechanical System
NP	Nanoparticle

ORR	Oxygen Reduction Reaction
Pb	Petabyte
ppm	Part per million
ps	Picosecond
SDLTS	Scanning Deep Level Transient Spectroscopy
SDD	Silicon Drift Detector
sr	Stearadian
S/TEM	STEM and/or TEM
STEM	Scanning Transmission Electron Microscopy
SXES	Soft X-Ray Emission Spectrometry
TEM	Transmission Electron Microscopy
TEAM	Transmission Electron Aberration-corrected Microscope
Tb	Terabyte
UHV	Ultra-High Vacuum
UV	Ultraviolet
WDM	Warm Dense Matter
W/EDS	Wavelength- or Energy-Dispersive X-ray Spectroscopy
XFEL	X-ray Free Electron Laser

Executive Summary

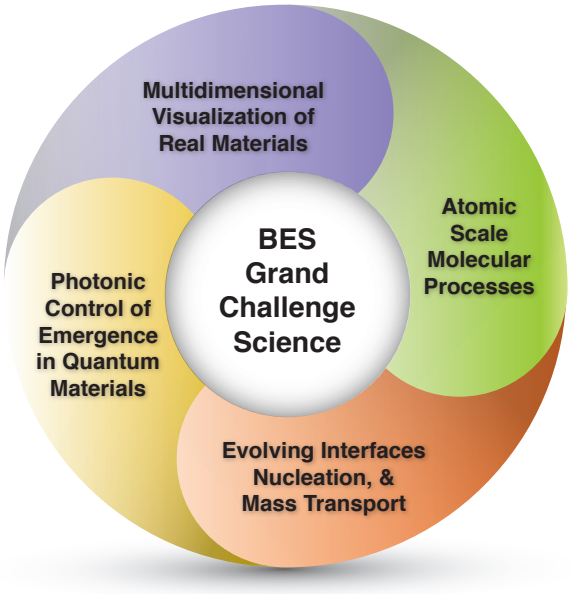
A two-day workshop on the Future of Electron Scattering and Diffraction, sponsored by the Office of Basic Energy Sciences (BES), was held on February 25-26, 2014 in Rockville, Maryland. The goal of the workshop was to identify the frontiers in electron scattering and diffraction that address Grand Challenges in chemistry, material science, physics, and biology. The workshop was organized in four topical sessions: Ultrafast Science, Advances in Imaging - Resolution and Tomography, Sample Environment and Hybrid Instrumentation, and Measuring Functionality.

The ability to correlate the atomic- and nanoscale-structure of condensed matter with physical properties (e.g., mechanical, electrical, catalytic, and optical) and functionality forms the core of many disciplines. Directing and controlling materials at the quantum-, atomic-, and molecular-levels creates enormous challenges and opportunities across a wide spectrum of critical technologies, including those involving the generation and use of energy. The workshop identified next generation electron scattering and diffraction instruments that are uniquely positioned to address these grand challenges. The workshop participants identified four key areas where the next generation of such instrumentation would have major impact:

A – Multidimensional Visualization of Real Materials
B – Atomic-scale Molecular Processes
C – Photonic Control of Emergence in Quantum Materials
D – Evolving Interfaces, Nucleation, and Mass Transport

Real materials are comprised of complex three-dimensional arrangements of atoms and defects that directly determine their potential for energy applications. Understanding real materials requires new capabilities for three-dimensional atomic scale tomography and spectroscopy of atomic and electronic structures with unprecedented sensitivity, and with simultaneous spatial and energy resolution. Many molecules are able to selectively and efficiently convert sunlight into other forms of energy, like heat and electric current, or store it in altered chemical bonds. Understanding and controlling such process at the atomic scale require unprecedented time resolution. One of the grand challenges in condensed matter physics is to understand, and ultimately control, emergent phenomena in novel quantum materials that necessitate developing a new generation of instruments that probe the interplay among spin, charge, orbital, and lattice degrees of freedom with intrinsic time- and length-scale resolutions. Molecules and soft matter require imaging and spectroscopy with high spatial resolution without damaging their structure. The strong interaction of electrons with matter allows high-energy electron pulses to gather structural information before a sample is damaged.

Imaging, diffraction, and spectroscopy are the fundamental capabilities of electron-scattering instruments. The DOE BES-funded TEAM (Transmission Electron Aberration-corrected Microscope) project achieved unprecedented sub-atomic spatial resolution in imaging through aberration-corrected transmission electron microscopy. To further advance electron scattering techniques that directly enable groundbreaking science, instrumentation must advance beyond traditional two-dimensional imaging. Advances in temporal resolution, recording the full phase and energy spaces, and improved spatial resolution constitute a new frontier in electron microscopy, and will directly address the BES Grand Challenges, such



as to "control the emergent properties that arise from the complex correlations of atomic and electronic constituents" and the "hidden states" "very far away from equilibrium". Ultrafast methods, such as the pump-probe approach, enable pathways toward understanding, and ultimately controlling, the chemical dynamics of molecular systems and the evolution of complexity in mesoscale and nanoscale systems. Central to understanding how to synthesize and exploit functional materials is having the ability to apply external stimuli (such as heat, light, a reactive flux, and an electrical bias) and to observe the resulting dynamic process *in situ and in operando,* and under the appropriate environment (e.g., not limited to UHV conditions).

To enable revolutionary advances in electron scattering and science, the participants of the workshop recommended three major new instrumental developments:

A. Atomic-Resolution Multi-Dimensional Transmission Electron Microscope: This instrument would provide quantitative information over the entire real space, momentum space, and energy space for visualizing dopants, interstitials, and light elements; for imaging localized vibrational modes and the motion of charged particles and vacancies; for correlating lattice, spin, orbital, and charge; and for determining the structure and molecular chemistry of organic and soft matter. The instrument will be uniquely suited to answer fundamental questions in condensed matter physics that require understanding the physical and electronic structure at the atomic scale. Key developments include stable cryogenic capabilities that will allow access to emergent electronic phases, as well as hard/soft interfaces and radiation-sensitive materials.

B. Ultrafast Electron Diffraction and Microscopy Instrument: This instrument would be capable of nano-diffraction with 10 fs temporal resolution in stroboscopic mode, and better than 100 fs temporal resolution in single shot mode. The instrument would also achieve single-shot real-space imaging with a spatial/temporal resolution of 10 nm/10 ps, representing a thousand fold improvement over current microscopes. Such a capability would be complementary to x-ray free electron lasers due to the difference in the nature of electron and x-ray scattering, enabling space-time mapping of lattice vibrations and energy transport, facilitating the understanding of molecular dynamics of chemical reactions, the photonic control of emergence in quantum materials, and the dynamics of mesoscopic materials.

C. Lab-In-Gap Dynamic Microscope: This instrument would enable quantitative measurements of materials structure, composition, and bonding evolution in technologically relevant environments, including liquids, gases and plasmas, thereby assuring the understanding of structure function relationship at the atomic scale with up to nanosecond temporal resolution. This instrument would employ a versatile, modular sample stage and holder geometry to allow the multi-modal (e.g., optical, thermal, mechanical, electrical, and electrochemical) probing of materials' functionality *in situ* and *in operando*. The electron optics encompasses a pole piece

that can accommodate the new stage, differential pumping, detectors, aberration correctors, and other electron optical elements for measurement of materials dynamics.

To realize the proposed instruments in a timely fashion, BES should aggressively support research and development of complementary and enabling instruments, including new electron sources, advanced electron optics, new tunable specimen pumps and sample stages, and new detectors. The proposed instruments would have transformative impact on physics, chemistry, materials science, engineering and technology and other fields.

Introduction

A two-day workshop entitled "Future of Electron Scattering and Diffraction" was held on February 25-26, 2014 in Rockville, Maryland. The overarching question of the workshop was "What are the scientific frontiers requiring advances in electron scattering and diffraction to address new science in Chemistry, Materials, Physics and Biology?". About fifty scientists and researchers from universities, national laboratories, and industry, participated. The agenda encompassed plenary talks and breakout sessions in four key topical areas: Ultrafast Science, Advances in Imaging - Resolution and Tomography, Sample Environment and Hybrid Instrumentation, and Measuring Functionality. The breakout groups submitted reports on scientific needs and instrument requirements, which formed the basis for this report.

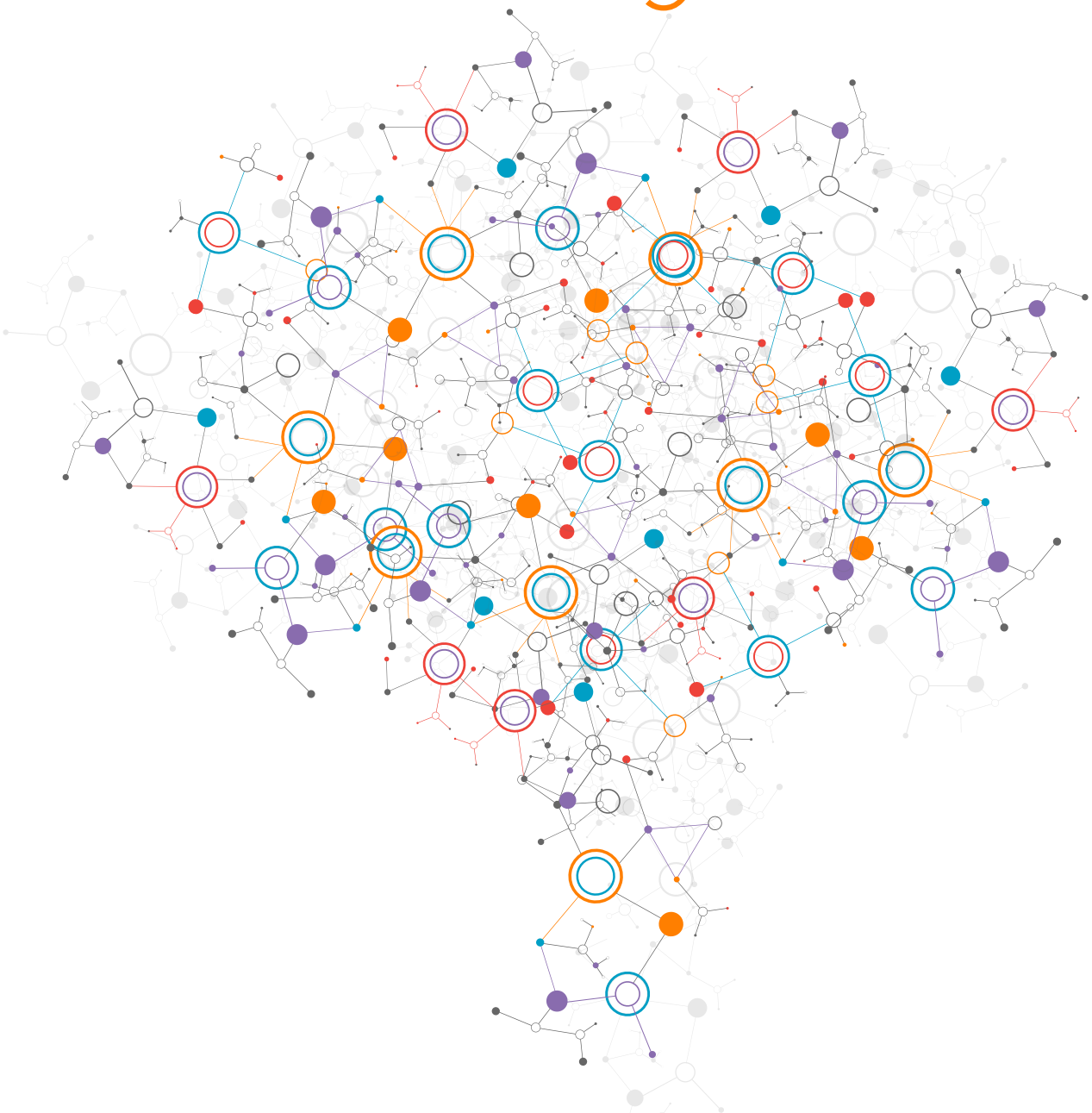
The Ultrafast Science Session discussed the potential of ultrafast electron diffraction, imaging and spectroscopy. Complementary to existing x-ray free electron lasers (FELs), ultrafast electron scattering techniques allow for understanding a wide range of phenomena from emergent behavior to chemical reactions and mesoscale science [Miller 2014, Spence 2012]. Exploring structural dynamics and behavior of matter under conditions far away from equilibrium were identified as high-priority goals. Details of the interplay between spin-orbit interaction and electron-lattice correlation in complex materials exhibiting fascinating properties will become accessible in the ultrafast regime.

Following the successes of the TEAM (Transmission Electron Aberration-corrected Microscope) project in imaging with unprecedented spatial resolution, the Advances in Imaging Session identified further possible breakthroughs in electron imaging in both physical and biological sciences. The session also identified the needs for further research, including understanding the existing physical limits on resolution, in order to identify the barriers to further improving spatial resolution [Uhlemann 2013].

The Sample Environment and Hybrid Instrumentation Session focused on enabling science, including nucleation, growth, and interfacial dynamics observed in gas, liquid, or other environmental electron microscopes. The Measuring Functionality Session discussed advances in instrumentation that are critical for enabling significant progress in measuring and understanding functional materials and grand challenges in condensed matter physics, including measurements related to electron correlations, polarization, magnetism, electronic phase behavior, collective excitations, phonons, hard/soft interfaces and surfaces behavior. Accessing and probing of new state of matter would require a stable stage design that can operate down to cryogenic temperatures with *in situ* and atomic resolution capabilities.

Recent developments in aberration-corrected electron microscopy, in new imaging techniques, along with revolutionary developments in detector technology and improved theoretical understanding have tremendously advanced the information that can be obtained from electron-scattering techniques. As summarized in this report, the participants of the workshop proposed a comprehensive vision for new and revolutionary advances in instrumentation over the next decade. Directly involving researchers who are the primary users, as well as experts from other fields, such as those in accelerator physics, source and detector design, were seen as critical for the United States to remain at the forefront of new instrument development in electron scattering techniques.

Key Breakthrough Science Opportunities and Challenges



A. Multidimensional Visualization of Real Materials

A.1 Electronic and Atomic Structure

In 1959, Richard Feynman challenged the electron microscopy community to build a better microscope that could identify all the atoms in a chemical structure. This challenge remains extremely relevant today. For example, the location of individual dopant atoms already controls the performance of current generations of silicon transistors and spintronic devices [Pierre 2010, Lansbergen 2008, Koenraad 2011]. Atomic-scale defects determine the optical and electronic properties of semiconducting and photonic materials, as well as mass transport in materials, such as lithium-ion batteries and fuel cells.

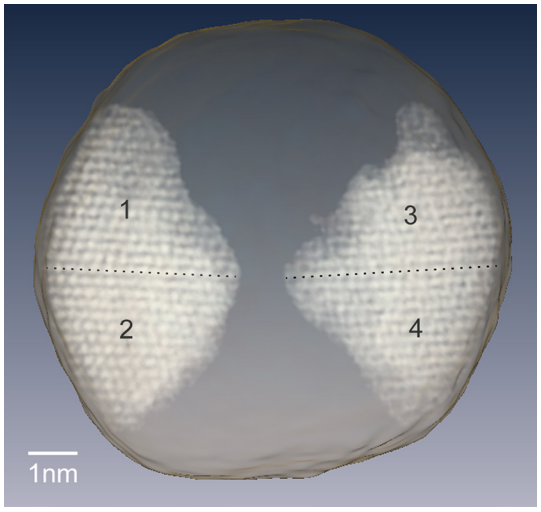


Fig. 1. *Identification of four major grains inside Au nanoparticle in 3-D [Scott 2012].*

Significant advances have been made in the imaging of individual impurity atoms inside crystalline materials using, atomic-number (Z) sensitive high-angle annular dark-field (HAADF) imaging and electron energy loss spectroscopy (EELS) in scanning transmission electron microscopy (STEM), including in three-dimensions [Voyles 2002, van Benthem 2006, Oh 2008, Okuno 2010, Couillard 2011, Bar-Sadan 2012, Krivanek 2010, Varela 2004, Gunawan 2011, Rossel 2012, Hwang 2013, Zhu 2013a]. These studies are typically carried out on relatively simple structures. In many engineering materials, defects form complex and non-uniform three-dimensional structures. For example, the Materials Genome Initiative promises to accelerate the discovery and design of new materials, but requires tools that can determine the structure and measure the properties of general grain boundaries, to fill the large gaps in the data sets needed for large-scale simulations. Determining the local structure, displacements, or atomic reconstructions around defects often involves a measurement accuracy of better than 1 pm, which is beyond current capabilities [Yankovich 2014]. Another unresolved challenge lies in the imaging of light atoms and vacancies. For example, understanding the insertion and removal of lithium atoms (Z = 3) in batteries is critical to advancing battery technologies needed for alternative energies and green transportation. Hydrogen storage involves the adsorption and desorption of hydrogen atoms (Z = 1) by diffusional processes, and clearly *in situ* observation of individual hydrogen atoms in metals, such as palladium, is an extremely difficult proposition. The oxygen reduction reaction (ORR) in solid-oxide fuel cells cathodes depends on oxygen transport aided by oxygen vacancies. Enhanced vacancy concentrations near oxide surfaces therefore play an important role in improving the ORR kinetics and lower fuel-cell operating temperature. A complete understanding of real materials requires knowledge not only of the local atomic configuration, but also of the electronic structure and vibrational modes in three dimensions (3D), and in many cases, how the structure evolves under external stimuli or in specific environments (Fig. 1).

Hybrid, correlative detection approaches that combine high-resolution electron imaging, EELS and x-ray spectroscopy with functional and transport measurements will allow direct probing of how individual defects affect materials properties. With Å-scale electron probes, the electronic and optical consequences of single atoms can be directly measured and mapped. Monochromated EELS could provide localized measurements of vibrational spectra and phonon modes, in addition to the optical absorption spectra from dopants, defects and interfaces identified by atomic-resolution imaging and core-level spectroscopic mapping. With atomically resolved secondary electron imaging [Zhu 2009], the chemical potential of surfaces may be mapped under bias. The development of electron emission spectroscopy may allow probing of Auger processes responsible for limiting the efficiency of light emitting diodes [Iveland 2013] or identifying the active sites in catalytic reactions. With the development of a stable, low temperature stage, cathodoluminescence could efficiently probe radiative recombination centers, correlating the light emission with the underlying physical and electronic structures revealed by EELS and elastic imaging. Similarly, under an electric bias, electron beam induced current (EBIC) imaging [Han 2014] and scanning deep level transient spectroscopy (SDLTS) could correlate individual defects with local band structure modifications, charge carrier lifetimes, and electron-hole recombination rates [Lang 1974, Breitenstein 1990, Progl 2008].

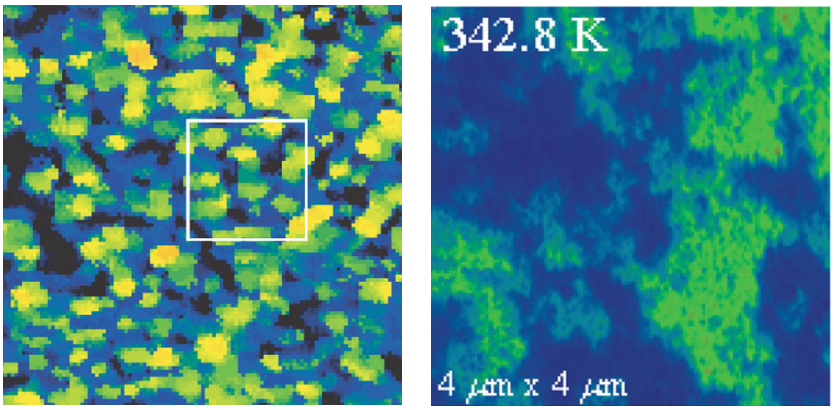


Fig. 2. *STM images of the superconducting gap (left, from [Lang 2002]) and metallic/insulating regions (right, from [Qazilbash 2007]). The left panel shows a 50 nm x 50 nm field of view. These images demonstrate the intrinsic electronic nanostructure of such materials.*

A.2 Collective and Correlated Phenomena and Materials

Properties of functional and quantum materials, such as magnetic, ferroelectric, multiferroic, or strongly correlated materials, are determined by collective and coupled interactions, such as strong Coulomb interactions among the electrons, strong electron-lattice (phonon) coupling, polarons, spin, charge and orbital ordering and fluctuations. These interactions are at the core of some of the deepest unsolved problems in condensed matter physics and give rise to extraordinary phenomena, such as high-temperature superconductivity, drastic changes in the resistance or tunable orbital, spin, and charge ordered states. Understanding, controlling, and manipulating these phenomena is of great importance for next generation information and energy technologies. It requires imaging of the real space atomic structure, spin and charge degrees of freedom, as a function of temperature, magnetic field, and external excitation. The unusual collective properties of the electrons in these materials are often governed by low temperature physics, such as quantum phase transitions. Furthermore, the electronic and atomic structure of these materials is usually highly non-uniform at nanometer length scales (Fig. 2). For example, they can exhibit highly complex charge-ordering phenomena, the coexistence of different electronic phases, and nanoscale

compositional and electronic fluctuations. The interaction between electronic phenomena and atomic-scale defects plays a critical but poorly understood role. For example, in high-temperature superconductors, the critical current can be doubled through engineering the defects that pin magnetic flux. Currently, the exploration of strongly correlated systems and their phase behavior as a function of external stimuli such as magnetic fields or pressure is mainly carried out using x-ray and neutron scattering methods, but *local* information about the material interior that is critical to the behavior is missing. Proximal probe approaches, including scanning tunneling spectroscopy, provide information on the local electronic structure and have revealed the intricate patterns of electronic phase separation, but are explicitly surface and near-surface sensitive.

Electron microscopy is the method of choice to explore the delicate links between structural distortions and electronic correlations. With appropriate energy and spatial resolution, combined information about atomic structure, electronic structure, and lattice vibrations will yield unprecedented knowledge of electron-phonon coupling, the effect of single defects onto electronic self-organization via structural distortion and electronic coupling, and the relevant length scales for electronic and photonic reconstruction at interfaces. In particular, enhanced energy resolution in EELS will not only enable the localized measurement of phonon spectra, bonding information, and electronic structure (including band gaps), but also lead to information on magnetic quantities, such as spin and orbital moments, through the study of the EELS near-edge fine structure. This will then allow studies of the structure, chemistry, bonding (mapping of charge and orbital reconstructions), phonon response, and magnetic properties of materials simultaneously and at the atomic scale. A main challenge is the energy resolution of EELS, which must be improved to below 10 meV. In parallel, high-brightness guns will be needed to maintain the required spatial resolution.

These advances must be combined with stable low/high temperature capabilities to allow these questions to be addressed at the relevant temperatures and phase spaces. Performing measurements at variable temperatures (across magnetic, structural, and superconducting phase transitions) will require an environment where atomic stability is reached quickly upon changing the temperature, from above room temperature to at minimum ~5K and preferably lower, with vibration and drift-free hold times of several hours at the operating temperature.

A challenge extending beyond Feynman's early vision is to develop atomic-resolution multi-dimensional (D) tomography (with D >3) to locate and identify all atomic species in complex systems, with additional dimensions such as time and with the control of temperature, external bias and sample environment. Such a powerful tool would have transformative impact on physics, chemistry, materials science, nanoscience and other fields.

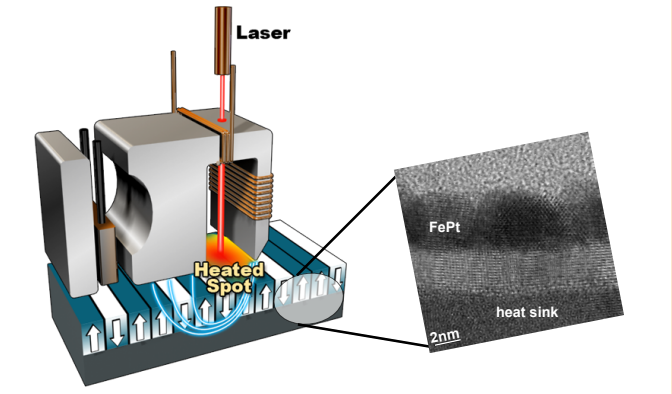


Fig. 3. *Schematic illustration of the envisioned next generation magnetic data storage devices where laser heating will assist reversal of the magnetic bit magnetization. An ultrafast local probe of the lattice can ideally determine the currently unknown energy transfer between FePt and heat sink layers. Figure courtesy of Gerardo Bertero.*

A.3 Energy Transport at the Nanoscale

Mapping the phonon density of states with atomic to nanoscale resolution, and correlating it with the structure of impurities, defects, local bonding, and interfaces that modulate the phonon spectra would provide information that is of extreme relevance for a wide range of materials, such as superconductors, thermal barrier coatings, nanoscale electronic devices, and thermoelectrics. For example, nanoscale heat transfer currently limits scaling of electronic devices and next-generation magnetic data storage (Fig. 3). Next generation thermoelectrics require materials with lower thermal conductivity to improve the Figure of Merit, which can be achieved using complex crystal structures or nanostructuring approaches [Snyder 2008, Wu 2013]. Being able to map phonon spectra in the vicinity of a "rattler" ion in a material or around a nanoscale inclusion would be of great importance.

A clear understanding of processes on picosecond timescales and nanometer spatial scales (e.g., phonon propagation and scattering at individual defects), would aid in designing thermal-transport properties [Cahill 2014, Biswas 2012]. At nanometer length scales comparable with the phonon mean free path, conventional heat diffusion based on Fourier's law does not hold and ballistic conduction becomes an important mechanism for phonon transport [Luckyanova 2012]. Broad science challenges include developing an understanding of the dynamics of energy dissipation in nanoscale materials, as well as accessing the crossover between the ballistic and the diffusive regime of heat and charge transport.

A pump-probe set-up with optical excitation would allow for depositing energy in the form of quasiparticle excitations at zero and finite wave-vectors. Utilizing atomic resonances or plasmonic field localization will enable the excitations to be spatially controlled. Ultrafast electron microscopy or nano-beam electron diffraction will then enable observation of the spatially resolved, real time energy transfer to various degrees of freedom. Such experiments will permit the study of heat conduction at nanoscale dimensions [Cahill 2003].

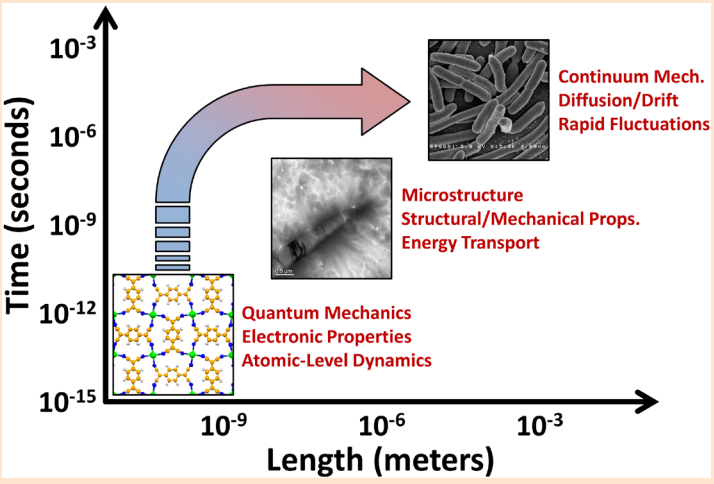


Fig. 4. *Length-time plot illustrating multiscale dynamics and how quantum-level properties emerge at the larger mesoscale described by continuum mechanics.*

A.4 Mesoscale Materials and Phenomena

The behavior of materials on the mesoscopic scale, ranging from nanometers to micrometers, is complex, scientifically compelling, and fundamental to a vast array of emerging technological applications. Examples include interface energetics, quantum confinement, protein dynamics, biological interactions, advanced materials synthesis and large statistical mechanical fluctuations—especially in extreme far-from-equilibrium regimes such as in warm dense matter (WDM)—all lead to unique behavior with no continuum-level analogues (Fig. 4).

The formation of mesoscale structures often involves processes on the microsecond scale or faster, well beyond the reach of conventional *in situ* microscopy techniques. For example, the crystallization of amorphous semiconductors, an important process for the development of new electronic, photovoltaic, and memory systems, has complex nucleation statistics and growth kinetics governed by the non-equilibrium initial structure.

Further, probing materials at ultrahigh temperatures and pressures will be critical for the understanding of WDM, which occupies a unique region of materials phases because of its tendency to be drastically transient and governed by highly nonreversible processes. The ideal experimental tool for studying this kind of mesoscale material dynamics must be capable of visualizing these processes, on their own natural length and timescales and under the physical conditions of the actual applications, producing sequences of directly interpretable real-space high-resolution images from very small volumes (μm as typical dimension) of material. Electron scattering is a natural choice for such a tool. High-quality electron lensing systems can readily produce images of multiple length scales, providing information not only about the atomic arrangement of the sample, but also about its morphology, composition, defects, and crystallography, precisely the structural variables most essential to performance.

B. Atomic Scale Molecular Processes

Atomically resolved imaging of molecules in soft matter and in chemical reactions could lead to major improvements in energy storage and utilization, potentially leading to the development of orders-of-magnitude better catalysts, streamlining reactive processes and allowing vast energy savings. For example, understanding chemical processes that occur on a catalytic surface requires atomic scale determination of the catalyst and reagent structures, as well as the interactions between them, including identification of the bonds that have formed and those that have broken [Ruan 2007]. This has so far only been achieved in a few cases with non-contact atomic force microscopy [de Oteyza 2013] (Fig. 5).

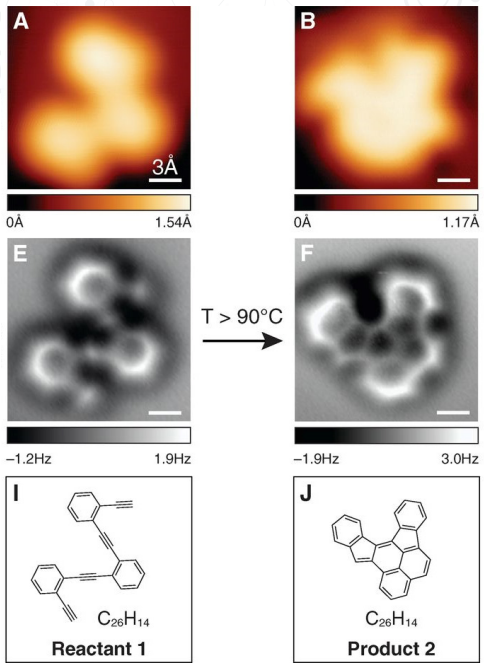


Fig. 5. *Non-contact atomic force microscopy images (center) of a molecule before and after reaction show dramatic improvement over images from a scanning tunneling microscope (top) and closely resemble the classic molecular structure diagrams (bottom) [de Oteyza 2013].*

Cryo-electron microscopy currently provides the only approach for imaging multi-component biological systems of at a spatial resolution approaching the nanometer scale. It allows visualization of large macromolecular machines both *in vitro* and *in situ* (i.e., in the cellular context). Such information is essential for understanding the structural basis of cellular function. Developments in spectrometer and detector technology that have taken place in the last five years allow for examining molecular functionality with limited spatial

resolution. The future challenge is to image and analyze molecular functionality with *both* high energy and spatial resolution without destroying the functionality through electron beam radiation induced damage. This requires the highest possible resolution under cryogenic conditions in an instrument that delivers the necessary high efficiency and integrated detection systems to ensure that the maximum possible signal is recorded for every electron. Energy-loss spectroscopy with higher energy resolution than what is possible today will allow molecular signatures to be investigated, with the intriguing prospect of exploiting the very low energy range of the spectrum (0-5eV) to obtain molecular signatures in the microscope with the specificity of techniques such as IR spectroscopy with sub-nanometer scale spatial resolution.

The time scales of bond breaking and formation in molecular and chemical processes are on a sub-100 fs timescale [Ihee 2001a, Gao 2013]. Real-time monitoring of chemical reactions became possible only with the advent of femtosecond lasers in the early 1980s. Femtosecond laser based transient optical spectroscopies have provided important insights into reaction dynamics. However, when applying these optical techniques to large and more complex molecular systems, formidable obstacles are encountered in linking the transient spectroscopy to the dynamics of nuclear motions. Ultrafast electron diffraction can measure interatomic distances with sub-Angstrom precision [Ruan 2004, Ihee 2001b] (Fig. 6). Not only can transient structural motifs be identified, but energetics of the excited states can also be mapped. In addition, ultrafast electron diffraction is suitable for low-density samples, such as those found in gas phase photochemistry.

Several prototypical cases of photochemical reactions have been investigated [Srinivasan 2003]. A prime example is the elucidation of the optically dark ring-opening structure in the so-called 'channel three' region in the photochemical reaction of benzene and pyridine [Lobastov 2001].

The ability to zoom in on intermediate structures may help engineer a specific photonic excitation effectively coupling to a molecular mode or modes that could promote a desired reaction process, thereby realizing quantum control of chemical reactions [Zare 1998]. The efficiency of a particular process depends on its speed compared to the rates of all available processes. For example, the polyene chromophore retinaldehyde in our eye transforms light energy into a special geometry change (isomerization). This is accomplished

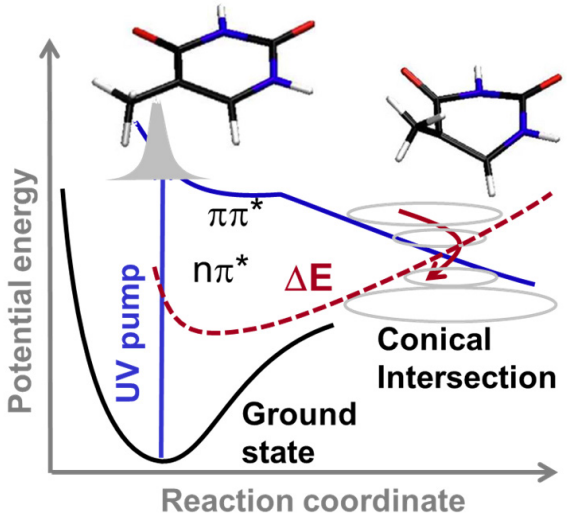


Fig. 6. *The relaxation of photo-excited thymine is a key process in DNA photo protection. Simulations indicate that the molecule relaxes through a conical intersection. The structures are from [Hudock 2007]. Figure courtesy of Markus Guehr.*

because the speed of isomerization is faster than the speed for heat creation of that molecule and its environment. The fastest, and therefore determining processes in energy conversion, cannot be described within the Born-Oppenheimer approximation [Domcke 2011, Yarkony 1996]. The combined determination of nuclear trajectories from ultrafast electron diffraction with electronic dynamics gained from ultrafast soft x-ray, including angle-resolved two-photon photoemission spectroscopy provides the possibility of obtaining a nearly complete picture of the molecular phase space upon photoexcitation. In addition, ultrafast electron diffraction from aligned molecules has enabled the application of diffractive imaging phase retrieval algorithms to reconstruct the molecular structure directly from the diffraction patterns [Hensley 2012]. In gas phase studies, the temporal resolution of ultrafast electron diffraction is currently limited to about 1 ps by the velocity mismatch between the optical pump and electron probe across the molecular jet. Major advances of femtosecond molecular imaging are on the horizon through a combination of high-energy probes, reductions in molecular beam size such as in microjet nozzles [DePonte 2008], or tilting the laser wave-front to reduce the velocity mismatch to below 100 fs.

Ultrafast electron pulses also have the potential to overcome the beam-damage-induced resolution-limit problem by enabling collection of data in the fs regime, which is likely faster than beam-induced damage, analogous to the "diffract-before-destroy" method in ultrafast x-ray crystallography [Chapman 2011].

C. Photonic Control of Emergence in Quantum Materials

Tailored photonic excitation of quantum materials offers the exciting opportunity of controlling a wide range of emergent materials and their properties. Recent groundbreaking examples include the emergence of room-temperature superconducting [Fausti 2011] (see Fig. 7) and metallic [Rini 2007] behavior from insulating phases through resonant excitation of lattice vibrations. The use of intense, single-cycle THz pulses, mimicking an electrical on-off switch relevant for applications (Fig. 7), caused the transition from insulating to metallic electrical transport in VO_2, a prototypical correlated oxide material displaying an insulator-metal transition in thermal equilibrium [Tao 2012, Liu 2012].

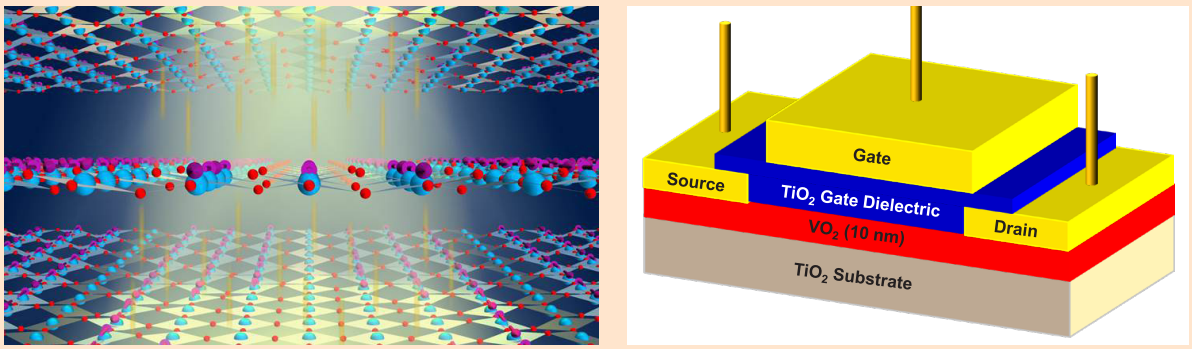


Fig. 7. *Schematic illustration of light-induced superconductivity in high Tc cuprates via ultrafast melting of stripe order (left). Ultimately the ultrafast electric field control of emergent behavior such as metalicity could lead to novel oxide electronics applications (right). Figures courtesy of Andrea Cavalleri and Stuart Parkin.*

Exciting the electrons from localized orbitals into delocalized bands with tunable mid- to far-infrared photons can provide subtle control of on-site Coulomb energy that may lead to a new pathway for ultrafast insulator-metal switching. Understanding and ultimately controlling the microscopic pathways that lead to such exotic behavior [Eichberger 2010, Zhu 2013b] will be one of the grand challenges and opportunities for materials physics in the coming decades.

Electron microscopy on a few nm length scales and sub-ps time scales will allow unprecedented insights into competing dynamical phases, coexistence or separation scenarios [Baum 2007, Qazilbash 2007], a question that is highly relevant to a very large materials class [Imada 1998, Ma 2014]. Intense single-cycle THz pulses are of particular interest as a unique means to examine the response to electric fields. Such studies are also of interest for the study of the switching behavior of multiferroic materials. The development of ultrafast electron nano-diffraction (sub-10 nm spot size) and microscopy opens up the possibility of complementary time-resolved imaging of nanoscale lattice dynamics using electrons to observe the coupled charge/lattice dynamics on the very length scales on which charge inhomogeneity has been detected in equilibrium (Fig. 2). Electrons provide simultaneous measurement of multiple Bragg orders, and have unique sensitivity to local electromagnetic fields, well suited for *in situ* functional imaging, such as probing vortex and ferroelectric domain dynamics with phase microscopy techniques.

The combination of stroboscopic ultrafast electron spectroscopy with nanometer scale imaging is uniquely equipped for observing the emergence of exciton-plasmon coupling at nanostructured interfaces. This capability is of great interest for utilizing collective excitations in metal-semiconductor interfaces, where the wave functions and electromagnetic modes of excitons and plasmons are strongly coupled [Kolesov 2009], leading to directed energy and charge flow. Spectroscopic imaging for mapping local plasmonic hotspots has been demonstrated based on photo-induced near-field enhancement [Yurtsever 2012]. Improving the temporal-spectroscopic resolution to the level of 100 fs – 100 meV could enable tracking of the detailed energy and charge flow for inspecting the plasmonic enhancement effect at its origin.

D. Evolving Interfaces, Nucleation, and Mass Transport

D.1 Interface Dynamics and Mass Transport

Interfacial dynamics govern the performance of the physical and chemical systems relevant to energy conversion, energy storage, biofuels, biomaterials, materials degradation, colloidal interactions,

synthesis, corrosion, oxidation, and catalysis. Despite their importance, interfaces in chemical environments remain enigmatic, and understanding their dynamic evolution represents a grand challenge in characterization.

Improved characterization of solid-liquid interfaces is crucial for practical applications, including the formation of the solid-electrolyte interphase in battery materials [Xu 2010, Gu 2013], materials growth in solution phase synthesis [Liao 2012, Zheng 2009, Li 2012, Yuk 2012], a mechanistic understanding of corrosion, or ion transport through membranes [Xu 2010].

At solid-gas interfaces, many fundamental questions remain: How do nanoparticle surfaces change in the presence of reactive gases [Nolte 2008, Deli 2010]? What are the local structures and dynamics of surface adsorbates on heterogeneous catalysts [Yoshida 2012]? What role do surface structures play in catalysis and oxidation [Yang 2012] and how does the material-reactant interface evolve [Zhou 2012]? What is the stability of nanoscale gas bubbles in the liquid phase? None of these questions can currently be answered by any atomic scale probe with reasonable temporal resolution. In many cases, *in situ* and *in operando* electron microscopy provides the only viable route towards addressing these issues. Triple-phase boundaries govern the kinetics of systems wherein ionic transport between two phases must be mediated by a process in the third. They dominate the performance of fuel cells, certain catalysts, nanowire and nanotube nucleation and growth, metal-air batteries, and some self-assembly processes. Discovery of new materials, novel functionality, and chemical processes depend critically on routine access to all phases of matter and the ability to capture the dynamic processes that occur at interfaces with high spatial and fast temporal resolution. The behavior of atomic species at triple phase boundaries has been notoriously difficult to elucidate. Further, interfaces often evolve during chemical reactions and control all the output of the chemical reaction. Therefore, the triple-phase lines, involving an additional transient phase at the interface, may essentially control chemical processing in nominally two-phase (e.g., solid-liquid) systems [Rodriguez 2007]. It is often observed that such a transient phase may be highly localized, extending over only a few monolayers.

In situ approaches also provide access to extreme environments under both equilibrium and non-equilibrium conditions. For example, hydrothermal and solvothermal reactions could be performed at high temperatures in enclosed environmental cells, providing new insights into metal-organic frameworks (MOFs) synthesis or hydrothermal conversion of biomass. In addition,

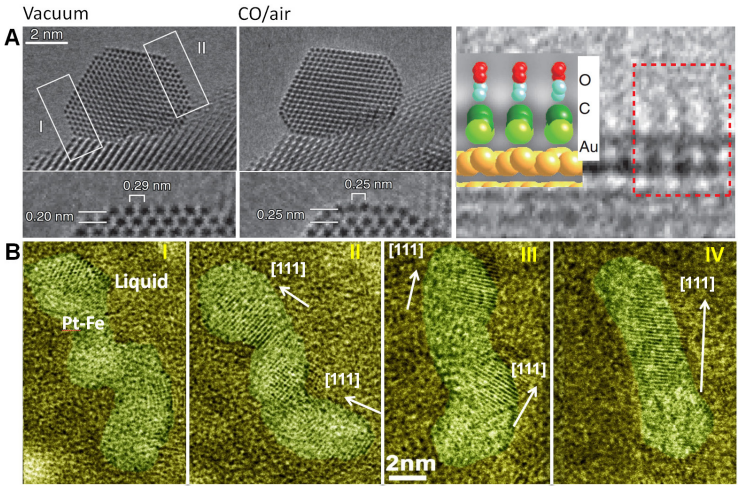


Fig. 8. *(A) Gas environmental TEM studies of Au nanoparticle (NP) catalysts supported on CeO_2. The inter-atomic distance of Au NPs in 1 Torr CO is increased in contrast to that in UHV. High magnification image of Au NPs with adsorbed CO matches the simulated image. [Yoshida 2012] (B) Real time imaging of Pt-Fe NP growth and shape evolution in a liquid solution of $Pt(acac)_2$, $Fe(acac)_2$ dissolved in oleylamine and pentadecane by liquid cell TEM. Surfactant ligands on the surface of Pt-Fe NP play an important role in nanoparticle interaction and shape evolution. [Liao 2012]*

low temperature chemistry could be performed to investigate problems like clathrate hydrate formation and stability. Reactions in hot and cold plasmas could also be investigated.

Understanding the response of atomic- and ionic-flows to macroscopic and microscopic gradients is of paramount importance for energy technologies, including batteries, catalysis, fuel cells, emerging information storage devices and novel materials synthesis (see Fig. 8).

For example, in some memristors, reversible electronically conducting channels form as a result of the motion of ions [Kwon 2010]. Channels may be as small as a single atom wide, and they have yet to be resolved. Real-space imaging of the motion of ionic defects or charged or uncharged vacancies is a key capability for addressing these science questions, in particular in combination with the ability to resolve the electric fields in and around these channels.

Correlating individual defects and defect interactions with materials properties is a great challenge due to difficulties associated with the characterization of individual defects under working conditions. For example, the movement of Li ions during electric biasing is accompanied by changes in lattice strain and transport of electrons (polarons), which can lead to the formation of defects such as dislocations, stacking faults and cracking [Fell 2013]. Nevertheless how these defects affect charge transfer, ion transport and stability of battery materials remains poorly understood due to the lack of atomistic-level characterization of the mechanism by which these defects are both generated and transformed during electrochemical operation.

D.2 Nucleation

Understanding of nucleation remains a critical fundamental issue in materials science, and improved control over nucleation processes, which can also lead to metastable phase selection, will have tremendous impact on a broad set of technologies. Nanostructured, metastable metals and ceramics, which tolerate high temperatures or high radiation flux have applications in improved efficiency of

turbine and future nuclear reactor designs. In electrochemical deposition, control of nucleation is essential for manufacturing coatings and structures, and for determining the grain size and surface roughness. Nucleation of features such as dendrites can limit the cycle life of batteries. The nucleation sites for oxidation or corrosion affect the mechanical behavior and lifetime of structural materials. Knowledge of particle nucleation from either liquid or surface adsorbate phases is needed to understand catalyst preparation, while information about nucleation of vacancy clusters is crucial to the semiconductor industry. In nanoscale systems, microscopy is the only way to obtain information about nucleation phenomena, since transformations are most often initiated by a single nucleation event [Zheng 2011].

Nucleation in liquids: Nucleation of solid Si from supersaturated liquid SiAu eutectic is particularly relevant to the initial stages of nanowire growth [Kim 2008]. The initial growth is rapid and allows super-saturation to be calculated (Fig. 9). However, subcritical fluctuations are not visible and the rapid initial growth is not captured. Spatial resolution in the 0.1 nm range would allow direct imaging of critical nucleus formation in this well-defined nanoscale system; analytical capabilities would allow compositional measurements during the phase transformation; and time resolution in the nano- to milli-second range (defined through considerations of diffusion at these length scales) would reveal kinetics with enough precision to understand the mechanism with the aim of controlling the transformation. Accurate knowledge of temperature and local pressure is essential. Liquid phase nucleation can be captured in the electron microscope using liquid cells, allowing nucleation events such as coalescence and sintering in liquid or at solid-liquid interfaces to be observed directly and growth mechanisms to be distinguished [Williamson 2003, Zheng 2009, Xin 2012, Li 2012, Liao 2012, Yuk 2012, Kimura 2014]. Capturing nucleation events of precipitates in liquids or at solid-liquid interfaces with high spatial and temporal resolution will allow improved fundamental understanding of nanomaterials synthesis, catalytic nanoparticle stability and electrochemical deposition, impacting the atomic-scale tailoring of such events to control materials properties.

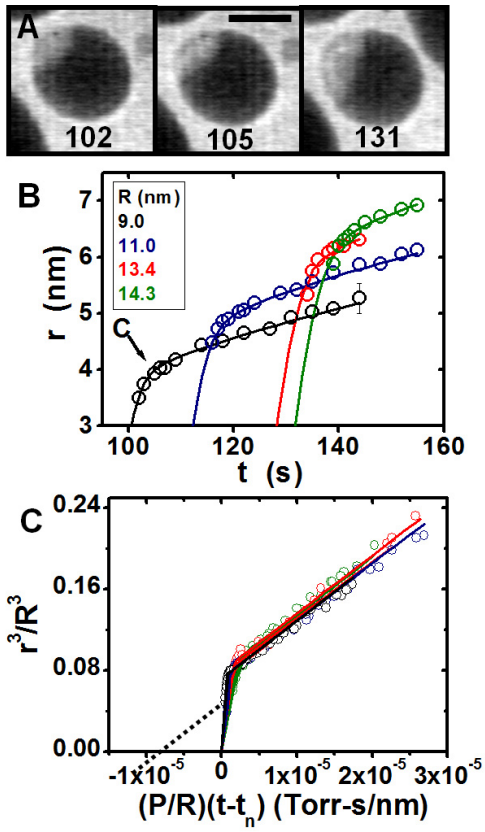


Fig. 9. *((A) Images of a growing Si nucleus (bright region) in a nanoscale eutectic droplet of AuSi (on SiN) during exposure to disilane. Disilane cracks on the surface, releasing Si into the droplet. When the Si super-saturation rises sufficiently, Si nucleates at the droplet periphery. Times in sec, 525°C, 4 × 10^{-6} torr, scale bar 10 nm. (B) Linear dimension r of several Si nuclei versus time t for droplets of different initial radius R (indicated in the box) during the same growth experiment. (C) Plots of r^3/R^3 versus $(P/R)(t - t_n)$ for all nuclei analyzed at 525°C and four different nominal pressures: 0.35 (black), 0.8 (blue), 1.5 (red), and 4.0 × 10^{-6} (green) torr disilane. t_n is the nucleation time. The jump size can be related to the super-saturation at t_n. [Kim 2008]*

Defect nucleation: The nucleation of defects such as dislocations is sensitive to local stresses and occurs too rapidly to capture at normal video frame rates. Dislocations nucleate at stress levels on the order of the ideal strength of a crystal [Minor 2006]. Since dislocations at near-theoretical strengths travel at the speed of sound, a comparable time resolution is required to capture their nucleation, motion, and the interactions between defects that control mechanical response. Heterogeneous nucleation of crystalline defects and cracks can depend on local stress concentrations or chemical inhomogeneities that are only accessible with high resolution electron microscopy and spectroscopy. For example, it is believed that stress-corrosion cracking is strongly influenced by the formation of thin interfacial films at the crack tip [Sennour 2009, Laghoutaris 2008, Guerre 2011]. However, questions remain concerning the mechanisms by which these interfacial oxides form and how they contribute to the dramatic reduction in fracture toughness. The ability to image the structure and chemistry of these films and the location of crack initiation and kinetics with atomic resolution, in a working environment, under stress, and at required speeds, would lead to fundamentally new insights in the important field of structural materials.

Table 1. *The four scientific opportunities that will be impacted by the advances in electron scattering strongly enable or enable the five BES scientific Grand Challenges.*

Science Opportunity	**Basic Energy Sciences Grand Challenges**				
Science Opportunity Impacted by Advances in Electron Scattering	Control Materials Processes at the Level of Electrons	Design and Perfect Atom- and Energy-Efficient Synthesis of New Forms of Matter with Tailored Properties	Understand and Control the Remarkable Properties of Matter that Emerge from Complex Correlations of Atomic and Electronic Constituents	Master Energy and Information on the Nanoscale to Create New Technologies with Capabilities Rivaling those of Living Things	Characterize and Control Matter Away Especially Far Away from Equilibrium
Multidimensional Visualization of Real Materials - Electronic and Atomic Structure - Collective and Correlated Phenomena and Materials - Energy Transport at the Nanoscale - Mesoscale Materials and Phenomena	Strongly Enabling	Enabling	Strongly Enabling	Strongly Enabling	Enabling
Atomic- Scale Molecular Processes	Strongly Enabling	Enabling	Enabling	Enabling	Strongly Enabling
Photonic Control of Emergence in Quantum Materials	Enabling	Enabling	Strongly Enabling	Enabling	Strongly Enabling
Evolving Interfaces, Nucleation, and Mass Transport	Enabling	Strongly Enabling	Enabling	Strongly Enabling	Enabling

Major Instrumentation Needs

The workshop identified a need for dramatically improved electron-scattering-based instrumentation to enable the scientific breakthroughs described in the previous Section. This Section discusses the specific instrumentation requirements and identifies potential technical solutions. It also discusses areas where more research is needed to overcome known technological barriers to further instrumentation development. The proposed instruments and the breakthroughs they enable are summarized in Table 2 at the end of this section.

A. Multi-Dimensional Atomic Resolution Electron Microscope

The vision for this instrument is to provide multi-dimensional, quantitative information over the entire real, phase, temperature, and energy space. Such an instrument will allow measuring structure, chemistry, bonding, phonon response, and magnetic properties of materials simultaneously and at the atomic scale. It will allow for three-dimensional visualization of dopants, interstitials, light elements and vacancies, mapping lattice vibrations and mass and energy transport, along with structure and molecular chemistry of organic and soft matter with atomic resolution. While developing this instrument will require significant investment, as well as overcoming engineering challenges, we do not believe that there are fundamental barriers to its realization.

This instrument will combine the following characteristics:

- Stable sub-1-Å resolution S/TEM
- Atomic resolution capability to at least 5K
- Modular specimen stage with *in situ* capabilities
- Post-specimen detectors to collect scattered electrons in full phase and energy spaces, and,
- Advanced detectors for spectroscopy.

Some of the details associated with this design are given below.

A.1 Sub-1-Å and Phonon Resolution at Below 5 K

To undertake measurements where the science is, an instrument that can measure structure and functional properties under conditions as close as possible to the natural state of a sample is needed. Low temperatures are currently inaccessible to advanced high-resolution electron microscopy and spectroscopy. Cryogenic temperatures also provide a benefit in stabilizing radiation and environmentally sensitive materials such as biological/inorganic interfaces or liquid/solid interfaces in energy storage materials, such as batteries and supercapacitors.

Stable sub-Å (Angstrom) resolution with *in situ* capabilities at low temperatures for extended time periods is required. Imaging performance should be at least comparable to today's room-temperature columns, but with a stable cold sample environment beyond what the current, holder-based technologies. Existing holders place the cryogen at the end of the holder rod, coupling uncorrectable vibrations into the image and creating excessive thermal drift. Such designs cannot provide sufficiently high resolution or stability for imaging and spectroscopy at the atomic scale. To go beyond

holder-based cooling requires cooling the sample from the objective lens area, allowing the cooling source to be more mechanically decoupled from the stage itself. Biological cryo-electron microscopes have demonstrated the necessary stability by cooling the entire sample environment via making column/polepiece cold, then using their large mass to provide mechanical and thermal stability. The cold environment has additional benefits as a cryopump, reducing both gas and sample borne contaminants, protecting reactive samples from oxidation or other environment degradations. The larger thermal mass would make it possible to maintain a stable low temperature with little or no sample drift or vibration for the 4-8 hours typically needed to align and record data. As discussed in Section A.2, low temperature may also improve the performance of advanced electron optics.

To access a wide temperature range, locally heating the sample, and measuring the temperature for stable feedback is needed, and could be provided by *in situ* MEMS technology. MEMS-based holders have a very small thermal mass and therefore quick response time, allowing the user to change temperature and have it stabilize rapidly, thus, enabling fast feedback for additional temperature stability. It would also allow for the possibility of heating to well above room temperature, possibly even temperature comparable to current MEMS holders of 800-1200 K. With electrical contacts needed for the MEMS heaters, additional possibilities for electrical biasing and other *in situ* experiments also become possible.

With such a diverse range of possibilities, a modular and flexible sample stage system is desirable. This would include options to apply magnetic fields; include a cryo-transfer system to keep samples clean when being transferred between different instruments; and different type of *in situ* holders. Here, the cryo-pumping has the benefit of ensuring very low partial pressures of oxygen and other contaminants. For many experiments, a wide (~10 mm) polepiece might be needed to allow very high-solid angle W/EDS. A field-free sample area would be needed for magnetic and superconducting experiments, which may limit resolution sufficiently that it must be a separate polepiece design.

Within the range of experiments envisaged, beam voltages would need to vary from 40-60 keV on the low end, to 300 keV, meeting the needs of both biological/engineering materials under representative conditions. Energy resolution will need to be improved below 10 meV. The ultimate goal is 1 meV spectroscopy capabilities. With the tradeoff between reduced beam current/increased spot size , the design of high-brightness guns should be revisited. At a minimum, a cold field emission gun with low energy spread (e.g., 0.35 eV or less) is desirable with W-based tips, but new designs with lower work-functions may improve this further.

A.2 Multi-Dimensional Signal Detection

The workshop identified a need for dramatically improved electron detectors that enable more efficient use of electron dose to the sample, and post-acquisition discovery of new signals and different aspects of scattering. Full position, momentum and energy collection will dramatically enhance the visibility of

point defects and other specimen parameters, such as internal electric polarization, by allowing for generating new contrast mechanisms. Conventional detectors (annular dark field and bright field detectors) do not allow for easy extraction of the signal as a function of position in the detector plane. Fully angular-resolved (**k**-space) information can be extracted from a single data set. The frontier is to develop high-speed pixel array detectors capable of measuring the energy as well as position of every scattered electron as a function of the 2D illuminating probe-scan coordinates. Such detector systems would enable reconstruction of any energy filtered, bright-field, or dark-field image and structure determination by matching to the entire I (**k**, E) data set.

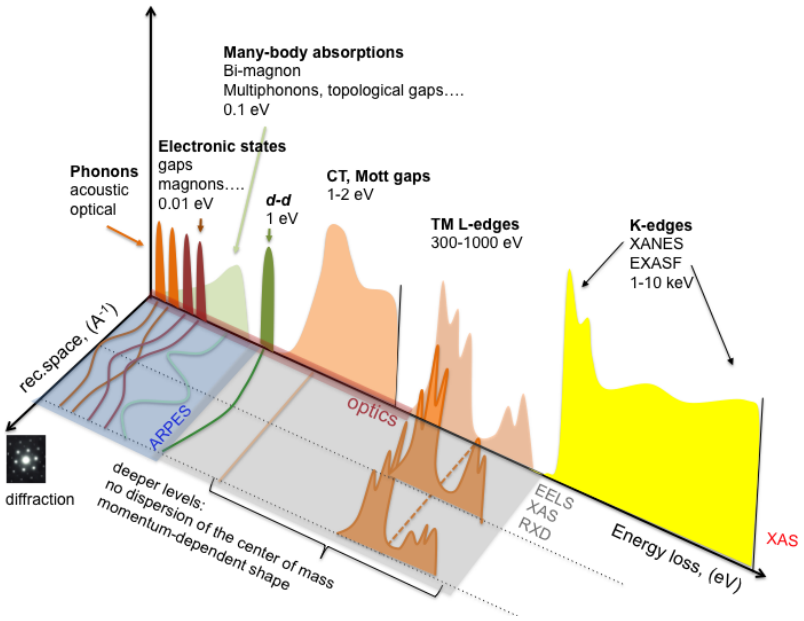
Full position-, momentum-, and energy-collection: In the first instance, the detector should be capable of full-frame readout at 25 kHz of at least 64 by 64 pixels, with single-electron sensitivity and detector quantum efficiency (DQE) no worse than existing direct-electron detection cameras. This is current state-of-the-art and can be realized now. In the medium term, a 256 by 256 detector with 1 MHz full-frame readout is highly desirable. This is an order of magnitude beyond the current state-of-the-art, and would require development. For energy-resolved detectors, the energy resolution must be <10 eV, and 1 eV is highly desirable. The pixel counts and readout rates should follow the same trajectory as the position-only detector. The technology to achieve this is not yet developed, which might involve superconducting transition detectors or narrow gap semiconductor junctions. This new detector will generate very large data sets, which will require new hardware and software developments. There must be real-time processing for rapid feedback during experiments and tools to synthesize various image signals post-acquisition. Finally, the large, rich data set provides opportunities for development of data mining and machine learning approaches to developing new, adaptive signals from the data instead of from *a priori* physical models and intuition.

4π energy-dispersive x-ray detectors (4π EDS): X-ray analysis is one of the most powerful atomic-resolution approaches to identify the elements present in a sample, but the signals are limited by physically restricted signal generation and poor signal detection configurations. Progress in addressing these limitations has been made with the latest aberration-corrected STEMs in combination with large solid-angle silicon drift detectors (SDDs) [von Harrach 2009, Ohnishi 2011]. It is now possible to acquire atomic-resolution EDS maps using these instruments. However, SDDs with collection angles of ~1 stearadian (sr) are still too low to obtain sufficient signals at the time scales accessible via ADF imaging and EELS, especially for thin samples and nanostructures. X-ray signals are generated toward an entire polepiece area of an instrument (4π sr); thus there is significant room for improving the collection angles in EDS.

High-energy resolution soft x-ray emission spectrometry: X-rays can, in principle, offer information about occupied density of states. In combination with EELS, the complete local electronic structure could be obtained. Currently, the energy resolution of x-ray acquisition by EDS detectors is as poor as 130 eV, which precludes obtaining any information about chemical states. An energy resolution of 1 eV or better is required. Such energy-resolution can be achieved by microcalorimeter-based bolometer EDS [Wollman 1997] or wavelength dispersive soft x-ray emission spectrometry (SXES) [Terauchi 2006].

The former suffers from very slow throughput and the latter requires relatively longer specimen-detector distance for better energy dispersions. Hence, both approaches end up with poor count rates and are not yet practical for routine measurements in S/TEM. Potential technical solutions include microcapillary and/or x-ray mirrors with redesign of detectors and instrument-detector interfaces.

Resolution beyond 50 pm: Over the past decade, BES-funded TEAM instruments have attained unprecedented spatial resolution of 50 pm. Continued improvement in the spatial resolution of aberration-corrected TEM instruments may allow for ever-more precise determination of atomic structure with the required contrast. Current aberration-corrected instruments have also highlighted challenges for achieving further improvements in resolution. For example, it was established that the atomic resolution of the TEAM 1 microscope was ultimately limited by vanishing contrast, which was shown to be due to image spread, meaning a loss of contrast caused by object shift relative to the final image detector during image exposure. Further research to determine the source(s) of these limitations has since pointed to magnetic thermal noise within every piece of metal in the microscope column [Uhlemann 2013]. A viable way to circumvent this noise is to cool down the environment of the electron beam, including the corrector as well as the objective lens, preferably to liquid helium temperature. The resolution-limiting Johnson noise would be roughly reduced by almost a factor of 10 on going from 300 K down to 4 K. Thus, to improve resolution below 50 pm, cooling of all elements of the correction system, as well as the objective lens and the object, might be required. As discussed in the scientific opportunities, the reduction in temperature of the important components (object, objective lens and corrector) would have additional advantages, such as much improved environment for specimen stability, reduction of thermal diffuse scattering of electrons, and greatly reduced beam damage for many materials. A spatial resolution of 0.25 Å is achievable theoretically at 300 kV. However, in addition to Johnson noise, other resolution-limiting sources in practice need to be evaluated.



B. Ultrafast Electron Diffraction and Microscopy Instrument

Ultrafast electron diffraction, imaging, and spectroscopy represent another grand challenge for modern electron microscopy, whilst offering a unique opportunity for understanding structural dynamics and the behavior

Fig. 10. *Taxonomy of excitations and their observability by pump-probe techniques. The different excitations are mapped on to the 3D space formed by momentum (reciprocal space), energy, and spectroscopic intensity. Courtesy of F. Carbone.*

of matter under conditions far away from equilibrium. The ultrafast pump-probe approach affords us a new means to discover the emergent properties of materials by tuning photon excitation energy in matter [Piazza 2014] (Fig. 10). Gaining knowledge of the dynamical behavior of exotic material systems requires characterization by tools that can observe structural details in relevant space scales (micron to angstrom) and time scales(femtosecond to microsecond). Conventional ultrafast electron sources with keV energies suffer from space-charge effects that limit the time resolution due to the temporal walk-off of the optical and electron pulses. High-energy (multi-MeV) electron sources can reduce these effects and provide access to larger sections of the momentum-space, accessing multiple Brillouin zones at the same time.

Given the capability demands stemming from these science cases, the ultrafast working group recommends an aggressive strategy for the development of an ultrafast electron diffraction and microscopy instrument that possesses the following capabilities:

- Ultrafast diffraction using the beam sizes from microns to 10 nm, to realize atomic spatial and 10 fs temporal resolution in reciprocal space.

- Single-shot real-space imaging with spatial-temporal resolution ranging from Å - μs to ~ 10 nm - ~10 ps.

A wide range of capabilities is included in between these two extreme cases for the new instrument characteristics and can be obtained by trading off the number of electrons per pulse, temporal/spatial resolution and the repetition rate. There are several key enabling technologies that will permit these needs to be met. These are described below.

B.1 Source and Electron Optics

A general theme that will enable the development of such a novel capability is high brightness beam generation (and preservation). This section has significant overlap with large ongoing research effort aimed at improving the photo-emitted electron beam characteristics for FEL-based light sources. Ultrafast electron sources are based on photoemission from solid-state cathodes. Employing advanced cathode materials and tuning the photocathode driver laser wavelength close to the material work function promises to lower the thermal emittance of the beams by nearly one order of magnitude. This will allow the utilization of larger source areas and a decrease in the electron density at the source

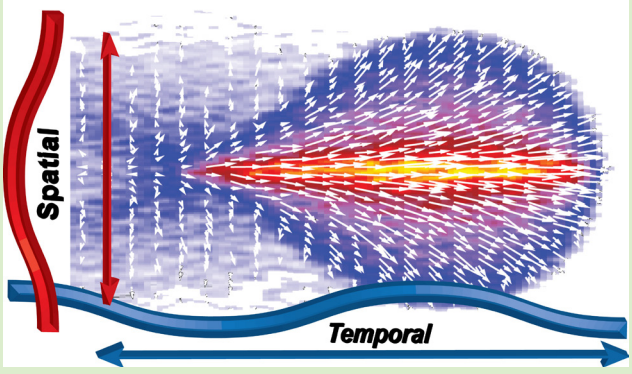


Fig. 11. *Free-space propagating ultrashort electron pulse exhibiting collective and stochastic space charge dynamics. The electron pulse manipulation using longitudinal and transverse lenses to reconstruct electron six-dimensional phase space allows optimization of combined temporal, spatial, and spectroscopic resolution.*

where the electrons are the slowest and the space charge effects have the largest detrimental effect on the beam quality [Portman 2013]: this will enable extremely low beam emittances and large relative transverse coherence lengths for ultrashort electron beams (Fig. 11). Since beam brightness scales at least linearly with the accelerating gradient on the cathode [Bazarov 2009], optimization of the gun gradient and geometry should also be considered in order to improve the brightness of the beams for the desired application.

Control of the transverse and longitudinal distributions, including the use of patterned photocathode, of the laser pulses illuminating the cathode will also be critical in improving the brightness of the source. Use of hollow cone illumination (a reciprocal mode of dark-field STEM) is another possibility to increase the source area and the number of electrons for single shot imaging applications, in order to avoid the time delay of scanning during image-formation. To meet the revolutionary spatial-temporal and spectroscopic resolution requirements, one will need to actively control the electron dynamics in six dimensions, by implementing various electron optics at different stages of pulse propagation.

The ultimate spatial, temporal, and spectroscopic performance must be optimized through the use of a series of optics, including multipole lenses and the correction of undesired aberrations (spherical, chromatic, and temporal). To advance ultrafast electron microscopy it is necessary to integrate tools for high-precision modeling of aberration corrections and handling high-intensity electron bunches to provide point-to-point simulation with detailed space charge dynamics and stochastic effects starting from the gun to the column and the detector.

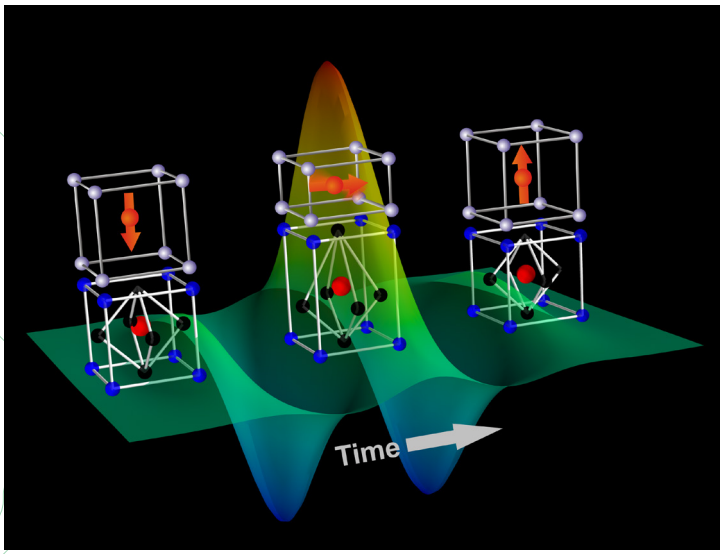


Fig. 12. *A single-cycle THz pulse coupling to ferroelectric polarization in a multiferroic material. The availability of such pump pulses will provide unprecedented opportunities for understanding and the ultrafast control of materials properties for use in the next-generation functional devices.*

B.2 Pump Technology

An important enabling technology, in particular for the control of emergent phenomena in strongly correlated electron systems, will be the availability of intense photon pumps, which are synchronous with the electron probe to ~10 fs time scales. The required photon pump energies span 1 meV to 5 eV, and would likely be provided by a range of sources, including linac-based sources and conventional laser technology. Ideal pumps would have the ability to have

both narrow band and broad-band modes of operation for different applications. In the optical and UV regimes, pumps provide non-thermal electron distributions. The use of XFEL radiation and THz pulses as a pump is appearing on the horizon as a radically new way to drive quasi-particle excitations and generate novel states very far from equilibrium (Fig. 12). In each case, it is crucial that the timing jitter between the pump and probe does not limit the temporal resolution of the experiment. This will require either a very stable source or time stamping capabilities or both.

C. Lab-In-Gap Dynamic Microscope

While the instruments described in the previous two sections represent major new instrumentation initiatives, it is also clear that another group of breakthrough science opportunities is related to much-improved capabilities for controlling the sample environment and conditions in sophisticated, dynamic ways. In addition to being a key opportunity area in its own right, advances in this capability will also be important to the instruments described previously.

The proposed instrumental solution to enable the *"Lab-In-Gap Dynamic Microscope"* concept takes advantage of several of the latest developments in the field of electron optics, variable electron source characteristics, sample environments, and enhanced detectors, to revolutionize our ability to capture and characterize dynamic processes at sub-Å spatial resolution and nanosecond temporal resolution. Integral to the approach is the exploitation of the latest in aberration-correction technology, developed under the auspices of the DOE BES sponsored TEAM project. The instrument would utilize spherical and chromatic aberration correction to increase the objective lens polepiece gap to ~10 mm, while maintaining sub-Å-scale image resolution in both TEM and STEM modes. Calculations of the contrast transfer function demonstrate that sub-Å imaging is feasible from such a configuration with an appropriate electron optical design. This significantly enhanced space will enable a multi-modal probing of the dynamics of evolving interfaces, an understanding of nucleation events, and of the effect of individual defects on materials' properties.

Importantly, the re-design of the objective lens region would allow for the incorporation of a substantial increase in the number and size of access ports for input of stimuli to the sample, as well as the proximity of multiple detectors localized to the sample. This has multiple, critical impacts on how the instrument can be utilized to accomplish forefront science. For example, it will significantly

enhance detection of electron beam induced signals (x-rays, photons and secondary-electrons) as well as improve manipulation and control of *ex situ* probes to stimulate dynamic processes. It also greatly enhances the ability to control the sample environment, allowing dramatic improvements in base pressure (to UHV) that can be concomitant with differential pumping apertures for environmental microscopy as well as closed-cell approaches for liquid-cell and super-atmospheric pressure microscopy and other forms of lab-on-chip experiments that exploit advanced micro-fabrication technologies. Versatile stage and holder geometry/design will allow the use of stable cartridge (e.g., biasing, cooling, heating stages) and/or side-entry sample holders (e.g., closed liquid/gas flow cells) depending on experimental variables. In this way, *operando* TEM/STEM (a subset or combination of various *in situ* methodologies) measures a technologically relevant functionality, simultaneously, can be directly correlated with evolving atomic level structure, composition, and bonding. For instance, the measurement of catalytic products generated inside the microscope during the observation of a catalyst in an environmental TEM is one example of the *operando* approach. Another example would be the acquisition of a charge/discharge curve during *in situ* cycling of a battery material. These *operando* approaches to *in situ* microscopy have the potential to allow functionally relevant structural motifs to be differentiated from spectator motifs that may form as a result of the application of *in situ* stimuli which do not contribute to the functionality of interest. Determining new ways to add *operando* capability to *in situ* TEM would maximize the impact of the dynamic Lab-In-Gap approach, and revolutionize our atomic level understanding of structure-function relationships.

EELS is currently undergoing a revolution in energy resolution with the recent development of monochromated STEM, offering energy resolutions approaching 10 meV [Krivanek 2014] and electron probes of 1 Å in size. Adapting this novel form of EELS with in situ gas and liquid-cell microscopy will provide a new tool for probing the chemistry of gas and liquid phases. It may even be possible to investigate adsorbate intermediate structures on the surface of a catalyst by exploiting the changes in the vibrational frequency when a gas molecule interacts with a surface.

To capture structural dynamics and evolving phenomena (such as nucleation events, defect and interface evolution, growth, and propagation) in energy-related materials, a range of temporal resolutions is needed [King 2005, Kim 2008, Flannigan 2010]. This approach would combine the latest advances in laser-driven photocathodes and sequential image acquisition, such as the movie mode, yet also be implemented such as to allow standard imaging approaches at the millisecond and below through utilizing direct electron detector (DDD) technologies.

Table 2 provides a summary of major instrumentation needs for enabling breakthrough scientific opportunities.

Table 2. *Summary of major instrumentation needs for enabling breakthrough scientific opportunities.*

<table>
<tr><th>Science Opportunity</th><th colspan="5">Instrumentation Needs</th></tr>
<tr><td colspan="6">I. Multi-Dimensional Atomic Resolution Electron Microscope</td></tr>
<tr><td></td><td>Sample environment</td><td>Energy resolution</td><td colspan="3">Full position, momentum and energy detectors</td></tr>
<tr><td>Phonon resolution</td><td rowspan="4">Stable sub-1-Å resolution S/TEM to at least 5 K

Low magnetic field environment

Straining, electric biasing, etc.</td><td rowspan="4">1 meV in EELS

1 eV in EDS</td><td colspan="3" rowspan="4">- Post-specimen detector with high-speed pixel array capable of measuring the energy of every scattered electron and their position with single-electron sensitivity;
- 256 by 256 detector with 1 MHz full-frame readout;
- 4π sr collection angle for EDS detectors.</td></tr>
<tr><td>Three-dimensional imaging of individual point defects</td></tr>
<tr><td>Correlating atomic and electronic structure with correlated phenomena, spin, and charge order at atomic resolution in operando</td></tr>
<tr><td>Characterization of radiation and environment sensitive materials at atomic resolution</td></tr>
<tr><td colspan="6">II. Ultrafast Electron Diffraction and Microscopy Instrument</td></tr>
<tr><td></td><td colspan="2" rowspan="2">Operation mode</td><td colspan="2">Spatial resolution</td><td rowspan="2">Temporal resolution</td><td rowspan="2">Number of electrons</td></tr>
<tr><td>Probe size</td><td>Reciprocal space</td></tr>
<tr><td>Photonic control of emergence in quantum materials</td><td rowspan="4">Diffraction / Imaging
Multiple shots / Single shots</td><td>10 nm</td><td>0.02Å</td><td>10 fs</td><td>10^3/pulse</td></tr>
<tr><td>Molecular dynamics in chemical reactions (gas, liquid and nanomaterials)</td><td rowspan="2">↕</td><td rowspan="2">↕</td><td rowspan="2">↕</td><td rowspan="2">↕</td></tr>
<tr><td>Energy transport at the nanoscale</td></tr>
<tr><td>Mesoscopic materials dynamics</td><td>0.1 nm</td><td>0.1 Å</td><td>1 μs</td><td>10^8/pulse</td></tr>
<tr><td colspan="6">III. Lab-In-Gap Dynamic Microscope</td></tr>
<tr><td></td><td>Larger polepiece gap</td><td colspan="2">Spatial and temporal resolution</td><td colspan="2">Hybrid instrumentation</td></tr>
<tr><td>Understanding the evolving interfaces and mass transport</td><td rowspan="3">10 mm pole gap with 1Å resolution</td><td colspan="2" rowspan="3">1Å and 1μs
or
1nm and 1ns</td><td colspan="2" rowspan="3">- Variable ports;
- Sample stage and holder design to allow measurements in liquids, gases, and plasma under stimuli;
- Sensitive detector;
- Sample-transfer systems</td></tr>
<tr><td>Control of nucleation</td></tr>
<tr><td>Correlating individual defects with materials properties</td></tr>
</table>

Additional Opportunities

Hybrid Instruments: The workshop also discussed hybrid concepts, such as between atom probe tomography (APT) and TEM. Such an instrument would overcome limitations in APT rather than electron scattering techniques. The former has at least two major physical limitations: a) Only about half of all atoms, independent of species, are currently detected; and b) uncertainties in the projection-law limit the spatial resolution for many specimens to 1 nm or more. A hybrid TEM/APT instrument has real potential to overcome the latter limitation by providing images of the specimen apex in an atom probe during the experiment. Atomic-scale tomography as envisioned here could: provide the 3D location of every atom with high spatial resolution; identify every atom, even isotopes, with high precision; generate images of a billion atoms (300x300x300 nm^3) in a few hours; offer high sensitivity analyses (1 atom/ppm); enable mapping of light elements in heavy element structures; and, address the need for dopant mapping.

Low KeV / Low Dose High Resolution TEM: One of the lessons learned from the TEAM project was that there is a great need for high performance imaging and spectroscopy at low accelerating voltages, such as for samples sensitive to beam exposure. Structural biology imaging with low dose techniques, and advanced electron detectors is currently undergoing a revolution [Li 2013]. In materials science, low doses are critical, for materials such as Li ion batteries, metal-organic frameworks, zeolites, or the delicate surface structures of catalytic nanomaterials. Improved performance of direct electron detectors at lower accelerating voltages is a necessary step toward damage-free imaging. Furthermore, the current generation of aberration correctors is not fully optimized for low voltage and low dose work. Critical advances are necessary in the long term stability of aberration correction electronics and power supplies to preserve the corrected state longer than the 3-5 minutes that is currently achievable at maximum resolution [Barthel 2013]. This is particularly important for low voltage electrons that are more strongly affected by the magnetic field perturbations.

Maximizing the field of view is critical to increase the experimental throughput. A larger imaging field of view dramatically increases the distance from the optic axis along which electrons in an image travel, and necessitates aberration correctors that are fully aplanatic over a field of view of at least 1 micron. The combination of aplanatic aberration-correction up to fifth order and a long correction lifetime would maximize the ability to image soft and hard materials at extremely low doses to avoid damage to specimens, and would fully leverage the capabilities of the next generation of large electron detectors with low voltage sensitivity.

Cross-cutting Areas

The workshop participants highlighted several crosscutting issues and opportunities that span all instrumentation needs that were identified. For example, as discussed in the sections above, *operando* studies are essential for understanding real materials and fundamental physical and chemical processes. The functional behavior of the material depends on the environment experienced while the material responds (e.g., reacting/deforming/catalyzing). A second broad underlying cross-cutting theme is that generating quantitative data is essential. This need requires not only generating quantitative images, spectra, or other data from the instrument, but also obtaining these data from specimens under precisely quantified conditions, such as temperature, environment, stress state, or the cumulative beam dose at, or experienced by, the specimen. Important crosscutting issues concern (i) the generation, handling, and processing of large amounts of raw data, (ii) the need for progress in theoretical understanding of electron-matter interactions, and, (iii) modeling and simulation. We discuss the second and the third issues in more detail below.

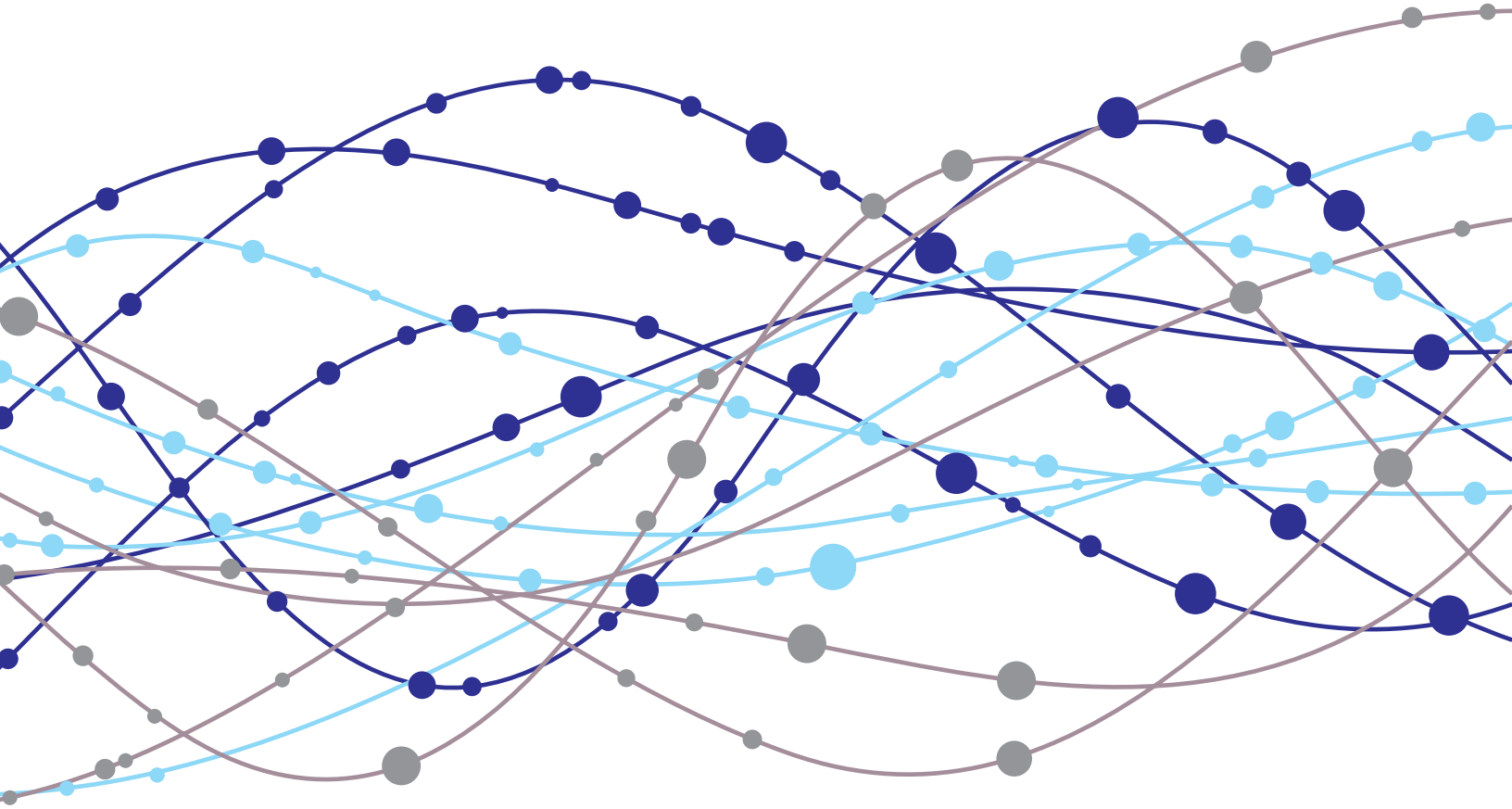
Data processing and storage: Realizing the key scientific opportunities provided by the advances in instrumentation described above will require high data acquisition rates, to minimize issues such as beam damage, limited sample or environmental stability, and the handling and processing of large data volumes. This may require different approaches to data acquisition, for example to acquire information with minimal redundancy using *adaptive measurement protocols*. For example "brute force" approaches of measuring atomically resolved EEL spectra on all slices of a tilt series would be inefficient, and involve beam doses that are unacceptably high for many samples. In addition to adaptive data-acquisition, fast direct-electron detectors are essential. To address the issue of extraordinary large data sets that are challenging to transfer, view, and analyze, algorithms could be developed to selectively store time sequences in which "significant events" are taking place. Computing resources, both fast hardware and suitable software and algorithms (i.e., expert systems, machine learning) are likely already available, but are currently underutilized in electron scattering and imaging. Data acquisition rates and storage needs for multi-dimensional tomography and/or ultrafast research could be very significant. The latest direct electron detectors can generate 4Tb during only 15 minutes of acquisition time, leading to annual data storage requirements that potentially could reach a few Pb (petabytes) per year. It is important that these challenges are addressed in a global, multi-facility fashion, rather than relying on local attempts to deal with this major issue.

As envisioned in the Materials Genome Initiative, state-of-the-art techniques in data science applied to materials experimental data hold great promise. Appropriately modified for electron scattering data, advances in signal and image processing of extremely noisy data sets may enable much more

materials information to be extracted per scattered electron, minimizing sample damage. New techniques in optimization applied to connect electron scattering data and simulations may generate solutions to otherwise intractable materials structures and problems.

Modeling and Theory: A closer link is needed between electron-optical observations and computational modeling. Experimentally measured microstructures, together with atomic resolution and temporal information could be used as input for simulations to forecast local behavior. Ultimately, optimized (i.e., sufficiently fast) simulations, using coarse-grained methods could possibly be linked in real time to *in situ* electron microscopy, e.g., to enhance temporal resolution by concentrating on sample areas where microstructural evolution is forecast as likely to occur. Advances in electron scattering capabilities will require concomitant developments in our ability to understand and predict electronic and vibrational excited state phenomena, and more, generally, the interaction between fast electrons and different states of matter. This facility requires theoretical frameworks and computational methods able to handle both ground-state properties and related many-electron interactions with excited states that may involve structural and orbital relaxations. Quantitative predictions for excited state phenomena pose a significant challenge for current theories, as are ground states of complex correlated systems. Progress in theory is needed to interpret electron energy-loss spectra, quasiparticle excitations and lifetimes, excited-state energy surfaces, transport properties, and related excited-state and collective phenomena. Leading edge measurements and synergistic theoretical efforts will enable advances in several disciplines.

Concluding Remarks



In summary, breakthrough science opportunities and the enabling instrumentation developments have been identified for the Future of Electron Scattering and Diffraction. It is clear that the world of probing matter with electron beams will experience revolutionary growth with the capabilities of ultra-small and ultra-fast imaging and spectroscopy, and with the ability to precisely control temperature, the environment (solid, liquid or gas), and the stimuli (e.g., electric field, magnetic field, light, and stress) of real-world samples. The breakthrough opportunities identified span a large spectrum, ranging from point defects to molecular dynamics, lattice vibrations, nucleation and growth, mesoscale dynamic phenomena, and more, each of which strongly impacts a broad range of sciences including materials science, chemistry, physics, and biology and directly connects to DOE Grand Challenges.

The proposed electron beam instrumentation development is directly related to enabling these breakthrough opportunities, and focuses on three key areas: multi-dimensional atomic resolution microscopy and analysis, ultrafast imaging and diffraction, and modular *in situ* and *in operando* dynamic microscopy and analysis. In parallel, cross-cutting areas in both science opportunities and instrumentation, such as adaptive data acquisition, and new processing, storage and modeling schemes, need to be developed which will complement and enhance these major instrumentation developments.

The proposed instrumentation moves the field beyond Richard Feynman's vision of "identify all the atoms in a chemical structure" to a new frontier of identification of atoms, dopants, and defects, understanding of their function and dynamics, and how real-world conditions and stimuli interact with and affect structure, properties, and processes at the sub-nanometer scale. The proposed instruments would complement other BES world leading science capabilities and result in transformative advances across fields of science and engineering that effectively address BES Grand Challenges and benefit Society.

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Appendix A: Workshop Agenda

Table A-1. *Tuesday, February 25, 2014 Agenda.*

Tuesday, February 25, 2014	
Tuesday AM - Welcome and Introductory Session	
8:00 AM	**Welcome from DOE BES** James B. Murphy/ George Maracas
8:15 AM	**Welcome from Organizers** Ernest Hall *(GE)*, Susanne Stemmer *(UCSB)*, Haimei Zheng *(LBNL)*, Yimei Zhu *(BNL)*
Plenary I: Ultrafast Science Session Chair: Yimei Zhu (BNL)	
8:30 AM	**Science Overview** John Spence (ASU)
8:50 AM	**Capabilities Overview** Chong-Yu Ruan (MSU)
9:10 AM	**General Discussion**
Plenary II: Advances in Imaging: Resolution and Tomography Session Chair: Ernie Hall (GE)	
9:20 AM	**Science Overview** John Miao (UCLA)
9:40 AM	**Capabilities Overview** Pete Nellist (Oxford U)

Tuesday, February 25, 2014		
10:00 AM	**General Discussion**	
10:10 AM	**Coffee Break**	
Plenary III: Sample Environment and Hybrid Instrumentation Session Chair: Haimei Zheng (LBNL)		
10:30 AM	**Science Overview** Frances Ross (IBM)	
10:50 AM	**Capabilities Overview** Andrew M. Minor (LBNL)	
11:10 AM	**General Discussion**	
Plenary IV: Measuring Functionality Session Chair: Susanne Stemmer (UCSB)		
11:20 AM	**Science Overview** David Muller (Cornell U)	
11:40 AM	**Capabilities Overview** Jian-Min (Jim) Zuo (UIUC)	
12:00 AM	**General Discussion**	
12:10 PM	**Buffet Lunch**	
1:20 PM	**NSRC & EBMC User Facilities Capabilities & Visions** Eric Stach (BNL)	Session Chair: George Maracas (DOE BES)
1:50 PM	**General Discussion**	
Breakout Sessions on Scientific Areas: What Science Needs To Be Addressed?		
2:00 PM	**Ultrafast Science** Breakout Chairs & members	Co-Chairs: Nigel Browning (PNNL) Xijie Wang (SLAC)
2:00 PM	**Advances in Imaging: Resolution and Tomography** Breakout Chairs & members	Co-Chairs: Bob Sinclair (Stanford U) David Smith (ASU)

Tuesday, February 25, 2014		
2:00 PM	**Sample Environment and Hybrid Instrumentation** Breakout Chairs & members	Co-Chairs: Peter Crozier (ASU) Shirley Meng (UCSD)
2:00 PM	**Measuring Functionality** Breakout Chairs & members	Co-Chairs: Igor Levin (NIST) David McComb (OSU)
4:00 PM	**Coffee Break, Reconvene Plenary Session**	
Summaries of Breakout Sessions on Science		
4:20 PM	**Ultrafast Science**	Breakout session representative
4:30 PM	**Advances in Imaging: Resolution and Tomography**	Breakout session representative
4:40 PM	**Sample Environment and Hybrid Instrumentation**	Breakout session representative
4:50 PM	**Measuring Functionality**	Breakout session representative
5:00 PM	**Day 1 Recap, General Discussion & Day 2 Expectations**	Organizers
5:15 PM	**Adjourn for Evening ** No Hosted Dinner**	

Wednesday, February 26, 2014		
8:30 AM	**Charge for Breakout Sessions on Enabling Developments for Electron Scattering & Diffraction Frontiers**	Organizers
Breakout Sessions on Enabling Developments		
9:00 AM	**Ultrafast Science Enabling Developments**	Breakout Session writers, Co-chairs, Organizers
9:00 AM	**Advances in Imaging: Resolution and Tomography Enabling Developments**	Breakout Session writers, Co-chairs, Organizers

Wednesday, February 26, 2014		
9:00 AM	**Sample Environment and Hybrid Instrumentation Enabling Developments**	Breakout Session writers, Co-chairs, Organizers
9:00 AM	**Measuring Functionality Enabling Developments**	Breakout Session writers, Co-chairs, Organizers
Summaries of Breakout Sessions on Enabling Developments		
11:00 AM	**Ultrafast science requirements**	Breakout session representative
11:10 AM	**Advances in Imaging: Resolution and Tomography**	Breakout session representative
11:20 AM	**Sample Environment and Hybrid Instrumentation Requirements**	Breakout session representative
11:30 AM	**Measuring Functionality Requirements**	Breakout session representative
11:40 AM	**General Discussion and Wrap-up**	Organizers
Workshop Adjourns		
12:00 PM	**Lunch**	
1:00 PM	**Charge for Report Writing Session**	Organizers
1:30 PM	**Writing Session**	Breakout Session writers, Co-chairs, Organizers

Appendix B: Workshop Participants

Table B-1. *BES Workshop Organizers and BES Program Managers.*

DOE Point-of-Contact
George Maracas *(Program Manager)* **Department of Energy** e-mail: George.Maracas@science.doe.gov
Organizers
Ernest Hall *(Co-chair)* **GE Global Research** e-mail: hallel@alum.mit.edu
Susanne Stemmer *(Co-chair)* **University of California – Santa Barbara** e-mail: stemmer@mrl.ucsb.edu
Haimei Zheng *(Co-chair)* **Lawrence Berkeley National Laboratory** e-mail: HMZheng@lbl.gov
Yimei Zhu *(Co-chair)* **Brookhaven National Laboratory** e-mail: zhu@bnl.gov
BES Working Group
Gregory Fiechtner Linda Horton Eliane Lessner George Maracas John Miller Raul Miranda James B. Murphy Jane Zhu

Breakout Sessions

The following picture shows some of the Ultrafast Group individuals participating in the Basic Energy Sciences Workshop:

Figure B-1. *Ultrafast Group.*

Ultrafast Science Group

Session Chair
Yimei Zhu *(BNL)*

Speakers
Chong-Yu Ruan *(Michigan State University)*
John Spence *(ASU)*

Co-Chairs
Nigel Browning *(PNNL)*
Xijie Wang *(SLAC)*

Breakout group
Jianming Cao (*Florida State University)*
Martin Centurion *(University of Nebraska)*
Hermann Dürr *(SLAC)*
David Flannigan *(University of Minnesota)*
John Hill *(BNL)*
Pietro Musumeci *(UCLA)*
Bryan Reed *(LLNL)*

The following picture shows some of the Advances in Imaging: Resolution and Tomography Group individuals participating in the Basic Energy Sciences Workshop:

Figure B-2. *Advances in Imaging: Resolution and Tomography Group.*

Advances in Imaging: Resolution and Tomography Group

Session Chair
Ernest Hall *(GE Global Research)*

Speakers
John Miao *(UCLA)*
Pete Nellist *(Oxford University, UK)*

Co-Chairs
Bob Sinclair *(Stanford)*
David Smith *(ASU)*

Breakout group
David Bell *(Harvard University)*
Uli Dahmen *(LBNL/NCEM)*
Max Haider *(CEOS, Germany)*
David Joy *(University of Tennessee)*
Tom Kelly *(Cameca)*
Peter Sutter *(BNL/CFN)*

The following picture shows some of the Sample Environment and Hybrid Instrumentation Group individuals participating in the Basic Energy Sciences Workshop:

Figure B-3. *Sample Environment and Hybrid Instrumentation Group.*

Sample Environment and Hybrid Instrumentation Group

Session Chair
Haimei Zheng *(LBNL/NCEM)*

Speakers
Andrew M. Minor *(LBNL/NCEM)*
Frances Ross *(IBM)*

Co-Chairs
Shirley Meng *(University California, San Diego)*
Judith Yang *(University of Pittsburgh)*

Breakout group
Peter Crozier *(ASU)*
Shen Dillon *(UIUC)*
Katie Jung Johann *(SNL/CINT)*
Karren More *(ORNL/ShaRE)*
Chris Regan *(UCLA)*
Eric Stach *(BNL/CFN)*
Chongmin Wang *(PNNL)*

The following picture shows some of the Measuring Functionality Group individuals participating in the Basic Energy Sciences Workshop:

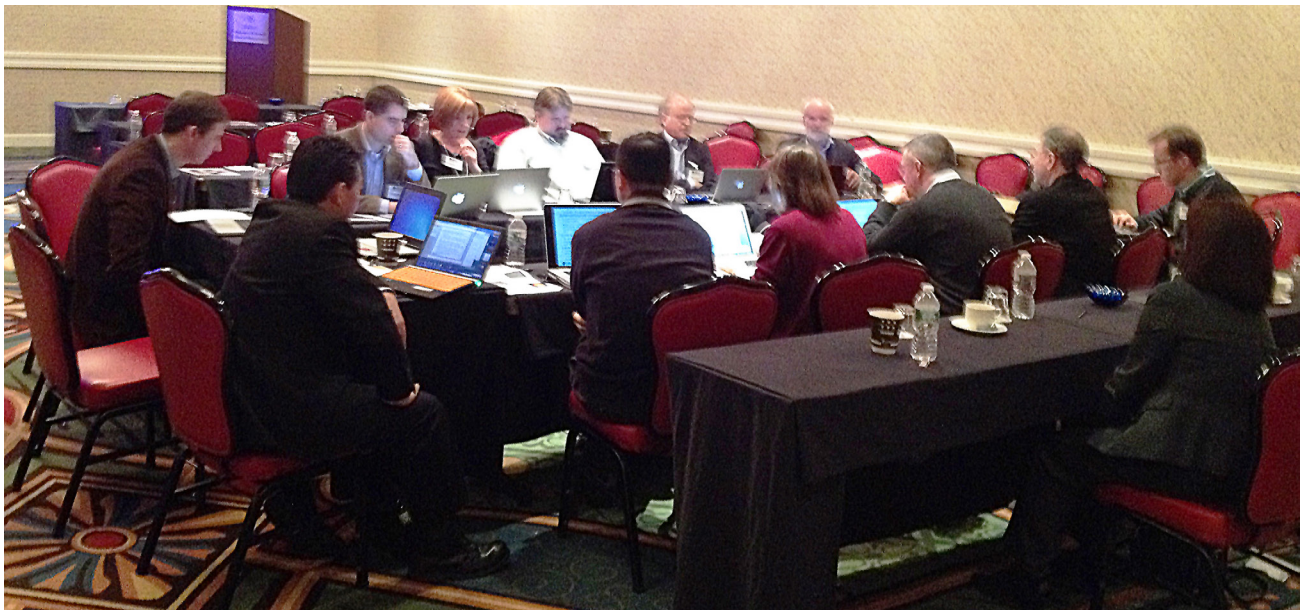

Figure B-4. *Measuring Functionality Group.*

Measuring Functionality Group

Session Chair
Susanne Stemmer *(UCSB)*

Speakers
David Muller *(Cornell)*
Jian-Min (Jim) Zuo *(UIUC)*

Co-Chairs
Igor Levin *(NIST)*
David McComb *(OSU)*

Breakout group
Barry Carter *(University of Connecticut)*
John Cumings *(University of Maryland)*
Richard Leapman *(NIH)*
Xiaoqing Pan *(University of Michigan)*
Amanda Petford-Long *(ANL/CNM)*
Paul Voyles *(University of Wisconsin)*
Masashi Watanabe *(Lehigh University)*

The following table provides the invited participants for the Basic Energy Sciences Workshop:

Table B-1. *Invited Participants.*

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Disclaimer

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