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1. Cover Page

Title: Theory and Simulation of Nanoscale Phenomena

Basic Energy Sciences: Scientific User Facilities Division, NSRC

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Funding Request (by year)

	FY16 ($K)	**FY17 ($K)**	**FY18 ($K)**	**Total ($K)**
Total	2,653	2,757	2,869	8,279

Human Subjects Use: No
Animal Subjects Use: No

Signatures:

Gary Grest, PI, SNL Date

Tanja Pietrass, Division Leader Date

Grant Heffelfinger, Director Date

2.0 Table of Contents

3.0 Tabular Budget and Staffing Summary

Total Budget and Level of Effort

Theory and Simulation of Nanoscale Phenomena

Total Operating Budget by Subtask

Requested Funding	FY16 ($K)	FY17 ($K)	FY18 ($K)	Total ($K)
Total	2,653	2,757	2,869	8,279

(Annual budgets cover loaded salaries, small purchases, postdoc salaries, and travel.)

Level of Effort

Key Personnel	FY 13 (FTE)	FY14 (FTE)	FY15 (FTE)
Frischknect	0.5	0.5	0.5
Grest*	0.75	0.75	0.75
Modine	0.5	0.5	0.5
Stevens	0.5	0.5	0.5
Tretiak	0.5	0.5	0.5
Trugman	0.5	0.5	0.5
Zhu*	0.6	0.6	0.6
Postdocs	2	2	2

*Thrust Leader and Partner Science Leader for Theory and Simulation of Nanoscale Phenomena

Materials and Supplies

Requested Funding	FY16 ($K)	FY17 ($K)	FY18 ($K)	Total ($K)
Total	225	250	275	750

4.0 Management Plan

4.1 Overarching Center Goals

The opportunities presented by nanomaterials are exciting and broad, with revolutionary implications spanning energy technologies, electronics, computing, sensing capabilities and biomedical diagnostics. Deriving the ultimate benefit from these materials will require the controlled assembly of diverse nanoscale materials across multiple length scales to design and achieve new properties and functionality, in other words, nanomaterials integration.

Integration has played a pivotal and revolutionary role in the development of nearly all science and technology. Perhaps the most familiar and dramatic illustration is the development of very large-scale integrated circuits where active and passive devices based on semiconductors, dielectrics, insulators, and metals are monolithically integrated on a single platform for specific applications. Even greater challenges exist as nanomaterials are integrated into new architectures to form functional systems. Interfaces and defects are formed whose structures and properties can dominate the chemical, mechanical, electronic and optical properties of the system. The effects of synthesis and fabrication processes on performance must be investigated and new directed- and self-assembly approaches developed for greater functional control. Combined bottom-up and top-down synthesis and assembly techniques must be optimized and/or invented to allow the intention design of hierarchical materials. Establishing the fundamental principles that underpin the integration of nanomaterials that display unique properties, such as quantum confinement, is of paramount importance to nanoscience and ultimately nanotechnology.

The goal of the Center for Integrated Nanotechnologies (CINT) is to plays a leadership role in integration of nanostructured materials to enable novel capabilities and applications through its function as a Department of Energy/Office of Science Nanoscale Science Research Center (NSRC) national user facility. By coupling open access to unique and world-class capabilities and scientific expertise to an active user community, CINT supports high-impact research that no other single institution could achieve – the whole of CINT including its user community is greater than the sum of its parts.

4.2 Overarching Thrust Goals

The overarching goal of the CINT Theory and Simulation of Nanoscale Phenomena (TSNP) thrust is developing and applying theory to understand and simulate, e.g., structural, electrical, magnetic, mechanical, thermal, and optical behavior of integrated materials and systems with nanoscale structure. The TSNP thrust is focused on identifying the fundamental underlying concepts that control structure and properties when nanoscale building blocks are integrated into a single composite system. The novel behavior of such systems appears as a result of the interactions between the components. Typically such systems involve competing interactions, which are controlled by and interact with the nanoscale structure of the system. Such competing interactions are responsible for such phenomena as self-assembly, coexistence of nanoscale domains of different phases, and emergent properties. The nanoscale structure of the integrated system provides freedom to control, tune, and optimize the behavior of integrated nanosystems. Thus, research into both the behavior of nanoscale components and the interactions between them is essential to the thrust. The size and complexity of integrated nanosystems, as well as the presence of competing interactions, pose challenges for current theory and simulation. The TSNP thrust meets this challenge by taking advantage of: (i) the broad range of expertise of the staff, which spans the range from quantum to classical interactions; ii) the development of collaborations with key users from the theory and simulation community who can provide needed expertise not currently available at CINT; (iii) our strong collaboration with experimentalists (CINT staff and users) to help provide critical insights and validation of new models, designs, concepts, and principles; and (iv) the high performance computing resources available at the labs to address the complexity of the systems. Where theoretical tools to address an important problem are not available, the thrust develops analytical and computational approaches that enable calculations for such systems. These theoretical tools are applied to physical systems of interest to CINT Users, the other CINT thrusts, and the general scientific community with the goals of understanding the fundamental principles determining the behavior of integrated nanomaterials and nanosystems and guiding

ongoing experimental work to optimize particular functionality or even achieve multifunctional and/or responsive materials and systems.

The work within the TSNP thrust can generally be organized into three TSNP science directions: (i) Hierarchical structure & dynamics in soft matter, (ii) Excitation and Transport in Nanostructured Systems, and (iii) Emergent phenomena at Surfaces and Interfaces. These science directions map roughly in a one-to-one fashion onto the three CINT Integration Science Questions, which demonstrates that together they form a basis for understanding the science of nanoscale integration. The hierarchical structure & dynamics in soft matter direction investigates how one understands and controls the interactions between nanoscale building blocks to assemble specific integrated structures. This work aligns closely with experimental work occurring in the Soft, Biological, and Composite Nanomaterials (SBCN). The excitation and transport in nanostructured systems direction investigates the effects of nanostructure on non-equilibrium phenomena including optical excitation and transport of, for example, energy, charge, and heat. It is aimed to find design principles that govern the conversion of optically generated excitonic excitations into electrical charges in hybrid structures, and optimize the figure of merit for the conversion between various energy and information forms under non-equilibrium conditions. The current work in this direction has focused on two important application areas: Energy Harvesting and Understanding Tunneling Experiments, which link with experimental work within the Nanophotonics and Optical Nanomaterials (NPON) and Nanoscale Electronics and Mechanics (NEM) thrusts. An important future focus within this direction is developing and applying models for excitation and transport in nanowires for energy applications and charge/spin transport through quantum single dots and arrays and their response to environmental conditions for quantum information, and also for the coupling between plasmons and excitons in nanoscales. The emergent phenomena in correlated electron and functional materials through interface engineering direction investigates systems in which competing interactions or exotic states in individual constituents can be tuned or coupled through the artificially engineered interfaces present in integrated systems. The focus is on two very different systems (correlated electron materials that exhibit emergent properties and compound semiconductor alloy surfaces including topological insulators and Dirac/Weyl semimetals and two-dimensional materials) with similar underlying physical phenomena. The work on emergent properties aligns well with optical probe experiments performed in the NPON thrust and with those on artificially structured complex oxides and semiconductors grown in the NEM thrust. As will be demonstrated in the Narrative below, all of the TSNP thrust science directions have strong connections to CINT User projects.

4.3 Staff Resources

The TSNP thrust is managed by Thrust Leader Gary S. Grest from the CINT Core in Albuquerque and Partner Science Leader Jian-Xin Zhu from the CINT Gateway in Los Alamos. This management structure is beneficial in ensuring clear responsibilities for thrust management activities while at the same time fostering close coordination and teaming across the thrust and enhancing CINT's in-reach into both Los Alamos and Sandia infrastructure. Within the same thrust, there is also a close collaboration between staff at the Core and Gateway.

The staffing in the TSNP thrust is composed of 7 CINT Scientists. Brief descriptions of key personnel and their research interests are included below (in alphabetical order) to illustrate how each member contributes to the scientific work of the thrust. (See Biographical Sketches for more in-depth descriptions of staff and activities). The diverse and complementary expertise of people involved in the thrust allows us to address a wide variety of problems.

Amalie L. Frischknecht (SNL, Core)- Amalie's research interests are in understanding the structure, phase behavior, self-assembly, and dynamics of complex fluids and nanocomposites, particularly polymer nanocomposites and charged polymers such as ionomers. She uses both molecular theory (self-consistent field theory, classical density functional theory) and molecular dynamics simulations to relate molecular and nano-scale features to material behavior.

Gary S. Grest, (SNL, Core)- Gary's research interests are in applying large scale simulations, both atomistic and coarse grained, to address problems in soft materials. The main emphasis of his work has been to identify the time and length scales which are most significant in the physical system and match them to those accessible by numerical simulation. His current research activities are focused on transport in ionic polymer, responsive polymer films, rheology of polymer melts and networks, mechanical and viscoelastic properties of polymer nanocomposites and nanoparticle assembly.

Normand A. Modine (SNL, Core)- Normand is interested in using computational techniques to research surfaces, interfaces, alloys, and defects and the interactions between these components in nanostructured systems. A key component of this research is the development of methodologies for bridging length and time scales from static and time-dependent quantum electronic structure calculations to reduced models (Monte-Carlo, classical atomistic, effective mass, and continuum models) at longer length and time scales.

Mark Stevens (SNL, Core) – Mark's primary research interests are in the simulation of soft matter including polymers, self-assembled monolayers, proteins, and nanoparticles. He uses both atomistic and coarse-grained models in molecular dynamics simulations to understand the connection between the molecular interactions and the system structure and properties.

Sergei Tretiak (LANL, Gateway) – Sergei's primary research interests are in the area of theoretical chemical physics, with an emphasis on electronic structure and spectroscopy of organic and inorganic electronic nanomaterials. Current research interests focus on theoretical studies of excited states and optical responses of photoactive organic and inorganic nanomaterials. Sergei develops quantum chemical approaches for efficient and accurate modeling of electronic structure, dynamics, charge and energy transfer in large molecular systems and apply these methods to different materials such as conjugated polymers, dendrimers, carbon nanotubes, biological light harvesting systems, donor-acceptor complexes, semiconductor quantum dots, and hybrid perovskite materials.

Stuart Trugman (LANL, Gateway) – Stuart's expertise includes pioneering research on dynamics of quantum systems, including confined geometries and response to ultrafast optical, infrared, and terahertz probes, the dynamics of electron-phonon coupled systems and quasiparticle dynamics. Current research activities include calculating the ground state, excited states, and dynamics far from equilibrium of coupled quantum systems, including electrons and excitons coupled to quantum lattice (phonon) degrees of freedom, and the interpretation and design of ultrafast optical and terahertz experiments.

Jian-Xin Zhu (LANL, Gateway) – Jian-Xin's expertise is in the dynamical mean-field theory, theory of quantum phase transitions in heavy fermion systems; electronic structure theory in strongly correlated materials; theory of impurity problems in strongly correlated electron systems; structure and properties in nanoscale electronic systems including complex tunneling junctions and interfaces. He is experienced in the theoretical analysis of scanning tunneling microscopy (STM), angle-resolved photoemission spectroscopy (ARPES), and ultrafast optical spectroscopy (UOS) experiments. His recent research focus is on the development of modeling and first-principles electronic structure theory for electronic, magnetic, and optical properties of complex nanocomposites/coupled 2D materials, and the development of ultrafast dynamics theories in complex materials.

4.4 Resources and connections across CINT

The TSNP thrust at CINT provides opportunities and synergies to conduct purely theoretical research that focuses on the development of a new theoretical understanding of the properties of materials at nanoscale. At the same time the thrust is focused on strong collaborations with the other thrusts and CINT users. Specific examples are:

Strong ongoing collaboration between J.-X. Zhu (TSNP) and J. Yoo (NEM) on charge transfer between conventional semiconductors and two-dimensional transition-metal dichalcogenides. This collaboration focuses on electronic and optical properties in the coupled functional composites.

S. Trugman and J.-X. Zhu are collaborating with A. Taylor and R. Prasankumar and Houtong Chen (NPON) on the theory of collective excitations and quasiparticle dynamics in the bulk correlated materials, e.g. multiferroics and colossal magnetoresistive materials. These materials exhibit intrinsic nanoscale inhomogeneities that need to be investigated.

S. Trugman and J.-X. Zhu are collaborating with Quanxi Jia (NEM) on the theory for optimizing the functionality by interfacing strongly correlated electronic materials, including transition-metal oxides. The collaboration focuses on the working mechanism for the improvement of magnetoelectric coupling in these engineered materials. Future important work will be extended to pillar-like and particular-like transition-metal oxide nanocomposites.

A. Frischknecht and M. Stevens (TSNP) are collaborating with D. Huber (SBCN) and CINT users to understand the connections between ionomer architecture, ionic nanoscale cluster morphology, and dynamics.

S. Tretiak (TSNP) is collaborating with S. Ivanov (NPON) and H. Htoon (NPON) on understanding surface ligand effects on the photoinduced dynamics in semiconductor quantum dots. Tretiak is also collaborating with S. Doorn (NPON) on electronic properties of chemically functionalized carbon nanotube and graphene materials and with J. Martinez (SBCN) on optical properties of emissive conjugated dyes and small nobel metal clusters.

N. Modine (TSNP) is collaborating with S. Ivanov (NPON) in understanding the growth of Ge_xSn_{1-x} quantum dots at compositions where the corresponding bulk alloy would not be stable.

4.5 Laboratory Complementary Resources and In-reach

Non-CINT DOE BES and LDRD funding provides a complementary resource that supports the ongoing research at Sandia and at Los Alamos.

S. Trugman is funded by the LDRD DR program on multiferroic response engineering in mesoscale oxide structures, which is focused on the properties of pillar-based nanocomposites in films; and meso-photonic materials for tailored light-matter interactions, which is focused on high temperature photovoltaic and nonlinear applications of metamaterials. The benefit of having these projects in parallel with CINT funding is that it allows us to apply theoretical advances made under LANL LDRD funding to nanoscale materials of interest at CINT.

A. Frischknecht is funded under BES in the “Adaptive and Reconfigurable Nanocomposites” subtask of the Molecular Nanocomposites project. In this project, Amalie is applying her background in classical density functional theory and self-consistent field theory of polymers to understand the phase behavior and interactions of polymer-coated surfaces and nanoparticles. In particular, this work will explore the interactions of responsive Janus nanoparticles, which is not part of the CINT proposal. Amalie is also funded under DOE-ASCR in the CM4 project (Collaboratory on Mathematics for Mesoscopic Modeling of Materials), in which she is working on electrokinetics of charged colloids. This project is synergistic with her research on charged systems at CINT but focused on different problems.

M. Stevens is funded under BES in the “Adaptive and Reconfigurable Nanocomposites” and “Active Assembly” projects. The nanocomposites project is exploring the basic science associated with the use of energy consuming, switchable, and/or responsive components to create programmable and/or reconfigurable nanocomposites. Mark is leading the theory effort to understand the nature of the connection between switching molecular conformations and the nanocomposite structure. This work involves modeling and simulation of molecular switching. In the active assembly project, Mark is leading the theory effort to understand microtubule assembly and dynamics. This work involves developing models of tubulin and other synthetic macromolecules, which is not part of the CINT proposal.

G. S. Grest is funded by SNL LDRD program to develop highly accurate hierarchal coarse grained models that will accelerate the computation of the properties of nanoparticle assemblies. The models developed with this funding directly benefit the multi-scale modeling effort in CINT.

S. Tretiak is funded by LANL LDRD program associated with investigation and design of optically sensitive high-energy explosives. Although this work shares a common general theme with CINT, optimization of physical processes targeting specific technological applications is different.

J.-X. Zhu is funded by LANL LDRD program associated with investigation and designing of rare-earth-free strong magnets and of mesoscale functionality with skyrmions, and by NNSA-ASC program focused on the calculation of the cold curves for the equation of state metals. The developed electronic structure simulation and modeling capabilities will directly benefit the CINT research.

4.6 Distinguishing Characteristic of the Thrust

Overall the TSNP thrust provides a balance and complementary skills in theory and modeling that allows in depth theoretical analysis and understanding of integrated nanoscale hard and soft materials and systems. The thrust is well positioned not only to develop theoretical understanding, but also to provide an active feedback in the design of experimentally relevant nanostructures. There are strong, active collaborations with both experimental and theoretical Users. In this role, the TSNP thrust has the unique ability to act as the “glue” that binds the three CINT experimental thrusts and external Users (experimental and theoretical) into coherent efforts capable of greatly accelerating the pace of scientific progress in integrated nanotechnology.

5.0 Abstract

The Center for Integrated Nanotechnologies (CINT) is a Department of Energy/Office of Science Nanoscale Science Research Center (NSRC), operating as a national user facility devoted to establishing the scientific principles that govern nanoscale integration. Nanoscale integration is defined as assembling diverse nanoscale materials across length scales to design and achieve new properties and functionality. The CINT Theory and Simulation of Nanoscale Phenomena thrust is the component of CINT dedicated to developing and applying theory to enable nanoscale integration. Our focus is on understanding and simulating the unique behavior of integrated materials and systems with nanoscale structure. This mission is achieved through collaborations with CINT Users, between thrust scientists, and with CINT scientists from other thrusts. Our research is focused on three science directions that together form the basis for integration at the nanoscale, namely (i) Hierarchical structure and dynamics in soft matter, (ii) Excitation and Transport in Nanostructured Systems, and (iii) Emergent phenomena at surfaces and interfaces. A broad spectrum of techniques is developed and applied including continuum fluid theory, atomistic and coarse-grained molecular dynamics simulations, static and dynamic electronic structure calculations, multiscale modeling, low-energy effective Hamiltonian methods, and perturbative and exact quantum many-body approaches. These tools are applied to physical systems of interest to CINT Users, the other CINT thrusts, and the general scientific community with the goals of understanding and controlling the interactions between nanoscale building blocks to assemble specific integrated structures, controlling energy transfer and other interactions over multiple length scales, and designing and exploiting the interactions within assembled structures to achieve new materials functionality.

6.0 Narrative

6.1 Background and Significance

In the sections below, we provide an overview of the scientific directions of the TSNP thrust, highlight our previous work, and provide detailed descriptions of our plans for the next three years. As most of our activities are—and will be—based on user interactions, specific user projects are referenced where appropriate.

6.1.1 Overview

The CINT TSNP thrust focuses on understanding and simulating the unique behavior of integrated materials and systems with nanoscale structure. This novel behavior appears as a result of the interactions between the components. The relative strengths of various interactions change as we move from the macroscale to the nanoscale, and phenomena that are negligible at the macroscale (e.g. quantum tunneling) can become dominant at the nanoscale. As interaction strengths change with length scale, competition between interactions can select intrinsic crossover scales at which the dominant interaction in the system changes. Such interaction crossovers can lead to spontaneous self-organization of materials including self-assembly and the formation of domains when the competing interactions are associated with different types of order. In integrated nanosystems, which combine dissimilar components, these intrinsic length scales can couple to naturally occurring or artificially imposed nanoscale inhomogeneity. Such coupling can lead to coexistence and/or frustration between different types of ordering and often results in emergent phenomena (remarkable behavior that currently cannot be predicted based on the properties of the individual constituents). For example, the contact between the insulators can create the metallic electron gas at the interface. Additionally, ferromagnetism can be induced in an antiferromagnetic multiferroic material when the latter is used to form a superlattice with a ferromagnet.

Interactions within and between the nanoscale components are the key to controlling integrated nanotechnology. The CINT TSNP thrust focuses on understanding and control of the role of novel and competing interactions in integrated nanoscale systems. The TSNP thrust strives to tackle the three science directions that together form the basis for integration at the nanoscale: (i) hierarchical structure and dynamics in soft matter, (ii) excitation and transport in nanostructured systems, and (iii) emergent phenomena at surfaces and interfaces. These science directions are the key challenges needed to address the CINT integration science questions: How does one (i) understand and control the interactions between nanoscale building blocks to assemble specific integrated structures, (ii) find the design principles that govern the conversion of optically generated excitonic excitations into electrical charges in hybrid structures for energy harvesting, and (iii) optimize the functionality by combining the intrinsic tunability of complex materials into hybrid architectures?

6.1.2 Hierarchical Structure and Dynamics in Soft Matter

The ability to propagate the intrinsically unique behaviors of nanoscale materials into functional materials and systems at the macroscale is one of the most challenging issues in nanoscience integration. Nature provides a vast array of blueprints by which this challenge can be achieved in soft materials. Our goal is to develop strategies that will enable the hierarchical assembly of individual nano-constituents to harness their collective or emergent behaviors.

The TSNP thrust works to understand and predict the behavior of hierarchical structure and dynamics of soft matter systems. In particular, our efforts focus on calculating the interactions in such systems and understanding how to control their structure and properties. Key TSNP scientists associated with this effort are A.L. Frischknecht, G.S. Grest, and M.J. Stevens. The main tool for studying these complex systems is the world-leading Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [1, 2], which we use to perform state-of-the-art classical atomistic and coarse-grained molecular dynamics (MD). Other statistical mechanics methods are also employed, such as classical density functional theory (c-DFT) and polymer self-consistent field theory (SCFT) [3].

Our ultimate goal in this area is to develop a fundamental understanding of the interactions among nanoscale components and how these interactions affect the overall functionality of the hierarchical

structures, thus leading to optimization and control by design. To expand the spatial and temporal ranges significantly, we will continue our development of coarse-grained models from the underlying atomistic models while maintaining key (molecular) chemistry.

6.1.2.1 Nanoparticle Structure and Assembly

At the heart of nanoscience is the assembly of new materials from nanoparticles (NPs) [4, 5]. Much is unknown about their assembly process and material characteristics. NPs are almost always coated with an organic monolayer to prevent them from aggregating and to help disperse them in most matrix materials. These organic ligands also provide a means to tailor the chemical properties of the NPs through organic synthesis. The overall properties of NP-based systems can therefore be readily tuned via controlling the NP size, shape, and chemical structure of the ligands. MD simulations are being used to characterize the structure of NP coatings and to understand how they control the effective interactions between NPs and the resulting structure of NP assemblies [6, 7]. MD directly reveals the structure of the coating, which is typically not accessible experimentally. This insight is particularly important for using NPs for sensors because the organization of the coating strongly affects the NP's selectivity and sensitivity [8].

6.1.2.2 Structure on the Nanoscale

Many soft-matter systems have an internal structure on the nanoscale, which strongly affects both the equilibrium and dynamic material properties. Often the structure is self-assembled and hierarchical with critical nanoscale components. Measuring structure and dynamics on the nanoscale tends to be difficult. Theory and simulation can frequently provide detailed information and insight at the nanoscale and can complement the experimental measurements that can be performed.

One broad example of structure on the nanoscale is the clusters formed by the association of ionic groups, which control the function of several classes of materials with potential uses, from clean energy and water purification to sensors and drug delivery. We have chosen to focus particularly on ionomers [9] (polymers that contain a small fraction of ionizable groups). Ionomers have interesting properties that are due to nanoscale clusters formed by the ionic groups. They are less well-studied than polyelectrolytes [10, 11] and are a useful class of materials both for applications [12, 13] and for developing detailed understanding of the links between nanoscale structure and material properties and dynamics. We have been especially interested in studying how the distribution and morphology of the clusters impacts the conductivity and electrolytic transport in ionomers. We have gained insight into the cluster structure and are developing the key architectural strategies to manipulate the association of ionic clusters into well-defined morphologies that will offer a new level of control of these materials.

6.1.3 Excitation and Transport in Nanostructured Systems

Nanoscale components must interact to be integrated into a functional system.. These interactions enable and control transport in an integrated nanosystem. Transport is strongly modified by the nanoscale structure of the system, and understanding these modifications is central to many applications of integrated nanosystems [14, 15]. Current efforts in this TSNP direction focus on understanding transport of energy, charge, and heat. Energy harvesting is one of the major potential application areas for integrated nanosystems [16, 17]. Excitation by photons and energy transfer by radiative and non-radiative processes are closely related phenomena [18], so theoretical studies can address many aspects of these phenomena in tandem [19]. Furthermore, CINT uses ultrafast optical spectroscopies to explore the behavior of energy harvesting nanomaterials, and the modeling of the relevant excited state behavior is a major complementary effort within the TSNP thrust. Likewise, understanding heat transport and conversion at the nanoscale is particularly important to optimizing the performance of integrated nanosystems [20]. The transport of charge in integrated nanosystems frequently occurs by tunneling processes, and these tunneling processes themselves provide a powerful and sensitive probe of system properties [21, 22]. Therefore, we consider modeling and interpretation of tunneling experiments as a second major application area within this science direction. Key TSNP scientists associated with these efforts are S. Tretiak, S. Trugman, N. Modine, and J. X. Zhu. The main tools for studying this area of research include the Non-Adiabatic Excited State Molecular Dynamics package [23], exact diagonalization method for polaron transport [24], scattering matrix [25] and Green's function approaches [26] for electronic charge and heat transport and local electronic structure modeling at nanoscale. We will now discuss our two targeted application areas: energy harvesting systems and understanding tunneling experiments in more detail.

6.1.3.1 Energy harvesting, non-adiabatic excitation, and quasiparticle dynamics

In the realm of energy related research, advances are limited by a lack of understanding of several fundamental processes: how light is absorbed, how excitations relax, what role phonon/vibronic mechanisms play through multiple excited states (intraband relaxation), and how charge separation phenomena occur. Understanding and control over these processes (photoinduced pathways) lie in the heart of our efforts to design functional photoactive materials for many technological applications (e.g. solar energy harvesting).

Transport is strongly modified by the nanoscale structure of the system. As the interactions between different degrees of freedom become stronger, composite excitations such as plasmons, excitons, polarons, and polaritons become important components of transport in nanostructures. Closely related to these composite excitations is the development of quantum correlations between different degrees of freedom. This is a key scientific phenomenon controlling excitation and transport in nanosystems. Work in this direction couples to the ongoing modeling of transport in nanodomains. We are developing methods to investigate correlation effects.

6.1.3.2 Understanding Tunneling and Transport Experiments

In addition to the energy transport mentioned in the previous subsection, carrier transport at nanoscale or through hybrid structures is also of interest. Operation of scanning tunneling microscopy is based on quantum tunneling of electrons. Due to the exponential dependence of the current on distance away from the surface, electronic and structural features can be mapped out with atomic precision, a resolution hard to achieve with other techniques. Extreme sensitivity makes STM a very powerful technique but also challenging to interpret, and theory and simulation are necessary in interpreting STM experiments. The TSNP thrust puts a focus on this area. Specific applications include the interpretation of STM experiments on graphene and other low-dimensional materials in a variety of settings. In parallel, the TSNP also focuses on the transport through graphene nanopores with biological molecules and the understanding of charge/heat/spin transport and conversion through tunnel junctions or contacts.

6.1.4 Emergent Phenomena at Surfaces and Interfaces

Competing interactions in integrated nanosystems can result in the formation of nanoscale domains, which can interact with natural (e.g. composition fluctuations in an alloy) [18] or artificial (e.g. in a heterostructure) nanostructure [19, 20]. Nanosized domains are particularly sensitive to the inhomogeneity associated with integrated systems. Even in cases where a homogenous system would have one uniform phase, integrated systems commonly upset the delicate balance between competing interactions and develop nanoscale domains. Such inhomogeneous systems often show frustration between different phases or types of ordering, and this can result in emergent properties [21].

In integrated nanosystems, nanoscale inhomogeneity is ubiquitous. Finite structures have surfaces, and integrated systems have interfaces. At the nanoscale, these surfaces and interfaces comprise a large portion of the system. One of the major challenges in understanding the behavior of integrated nanoscale systems is that the structure of these surfaces and interfaces is generally unknown and may differ substantially from the structure of constituents. We will now discuss these examples of emergent phenomena at surfaces and interfaces in more detail.

6.1.4.1 Emergent Properties in Correlated Electron Heterostructures

Emergent properties provide the most dramatic examples of competing interactions in complex materials. These competing interactions are associated with different types of order (e.g. orbital, magnetic, ferroelectric, and superconducting). When they interact in an environment of natural or artificial nanostructure, dramatic new properties of materials, from colossal magnetoresistance, and relaxor ferroelectricity to perhaps even high-T_c superconductivity and multiferroic phenomena, can emerge. Competing interactions and ordering modify the dynamical behavior of the system and can be probed using various spectroscopic techniques. We have been focusing on planar-like transition-metal oxide heterostructures, in which the balance of competing interactions is controllably perturbed. In the long term, we will develop novel simulation and modeling tools that allow us to understand and design novel properties of 3D integrated nanostructures involving correlated electronic materials. Zhu has been

developing new theoretical techniques that incorporate electronic correlations to understand the emergent properties in transition-metal oxide heterostructures and nanocomposites. Trugman has been developing understanding of transient behaviors in both bulk and composite materials.

6.1.4.2 Semiconducting Compound Surface and Interface Structure

Surfaces and interfaces typically involve interrupting the bonding patterns of the constituent materials. They not only tune the competing interactions in strongly correlated materials, but also frequently reconstruct in semiconductor compounds in order to eliminate dangling bonds and reduce the energy cost of this disruption in bonding. The specific atomic structure of this reconstruction is determined by competition between local chemical bonding and long range electrostatic and strain interactions. Furthermore, thermal fluctuations and variations in composition can lead to nanoscale inhomogeneity in the structure and morphology of the surface or interface. In certain cases, long range electrostatic and strain interactions can even lead to the formation of nanoscale domains of different structures. The structure of reconstructed surfaces can be observed by a variety of experimental techniques, and thus considerable information about structural patterns can be obtained by comparing the results of simulations and experiments for surfaces. In contrast, it is much more challenging to observe the detailed structure of interfaces experimentally, and reliable theoretical predictions would be highly valuable in understanding how interfaces determine the behavior of integrated nanosystems. TSNP scientist Modine has worked with CINT users to develop tools to systematically identify the structure of surfaces and interfaces

6.2 Progress Report

TSNP thrust work has involved a complementary combination of user-driven science and CINT science. The majority of our work can be viewed within the context of the thrust science directions discussed above. This demonstrates our ability to maintain a coherent science effort despite the diverse needs of users, while allowing the development of new capabilities to impact future user needs. We will now discuss the progress that we have made to date for each of the thrust science directions.

6.2.1 *Hierarchical Structure and Dynamics in Soft Matter*

We have continued to make significant progress on the structure and dynamics of hierarchical soft materials including NP structure and assembly and structure on the nanoscale. Studying a range of physical systems allows us to address the major scientific questions relevant to integration and allows us to address the needs and interests of a diverse set of users.

6.2.1.1 Nanoparticle Structure and Assembly

Thin membrane films composed of a single layer of inorganic nanocrystals coated with organic ligands are currently of great interest for a range of applications from nanosieves to electric, magnetic, or photonic devices and sensors [27, 28]. Although these membranes have been found experimentally to be flexible yet surprisingly strong under indentation, the underlying microscopic origin of their large tensile strength remains unresolved. Using multimillion atom large-scale MD simulations, we probed the fundamental mechanisms underlying the unique mechanical strength of two-dimensional alkanethiol-coated gold NP membranes [6, 29-31]. Replicating experimental conditions [32, 33], NP membranes were formed at a water-vapor interface, and then the water was removed to form free-standing membranes. Mechanical tests of the resulting membranes showed that interactions between ligand end-groups (see figure 1) play a dominant role in determining membrane strength and stiffness. The ligand end-group also affects how these membranes fail under tension.

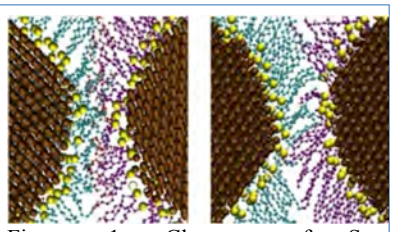

Figure 1. Close-up of S-$(CH_2)_{11}COOH$ terminated (left) and S-$(CH_2)_{11}CH_3$ terminated (right) Au NPs. H atoms are omitted except in the COOH end group. Carbon atoms are cyan on the left NP and purple on the right.

Nanoparticles in aqueous solution can be highly charged, and their dynamics depend strongly on interactions with ions in solution. Stevens and Frischknecht, guiding CINT postdoc M. Salerno [34], have investigated the underlying physics of highly-charged NPs in realistic solution conditions in the intermediate regime between the strong-coupling and Poisson-Boltzman n limits, where attractive

interactions between like-charged nanoparticles are possible. We examined the effect of NP diameter and charge, counterion valence and salt concentration on the interactions between two NPs and mapped out the conditions where divalent counterions yield attractive interactions (monovalent counterions only yield repulsive interactions as expected). For divalent counterions, highly correlated condensed layers of counterions form on the nanoparticles. As the separation between the nanoparticles becomes close to where the condensed layers would overlap, the interaction becomes attractive. We showed that non-monotonic behavior in the strength of the attraction is due to geometric constraints of counterion packing around the nanoparticles.

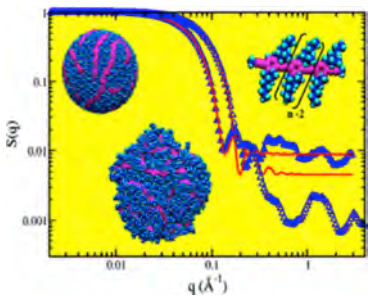

Figure 2. Images of the monomer chemical structure and polydot as made and in equilibrium in water. The data is the static structure factor S(q) for polymer substituted (▲) and without (open triangle) side chains in water with best fit to a fuzzy spherical form factor (solid lines).

We also studied a new class of light-emitting-and-absorbing soft NPs, known as polydots, which are formed by collapsing conjugated polymers into long-lived, nanometer size, globules as shown in figure 2. The luminescence characteristics of polydots differ significantly from those of spontaneously aggregated conjugated polymers, pointing to a new conformation of the rigid polymers in confined geometry. Grest and CINT user D. Perahia [35-39] resolved by MD simulations the internal structure of polydots, overcoming the challenge of probing structure within very small volumes. The simulations showed that while the chains are not in their equilibrium conformation, they remain predominantly spherical and compact in water and are stable over astounding long times even though they are not cross-linked. This work has opened the way to explore internal structures of soft nanoparticles that in turn will impact the design of new nanoparticles with well-defined luminescent characteristics.

In related work, Grest, in collaboration with CINT users S. Kumar [40] and M. Rubinstein [41, 42], studied how the addition of NPs affects the properties of polymer nanocomposites [43-46]. We showed that NPs always reduce the number of entanglements in a polymer melt, with this effect only becoming pronounced for small NPs or for high concentrations of large NPs.

Frischknecht continued to study nanoparticle assembly and behavior. In collaboration with CINT user R. Composto [47], she used self-consistent field theory to predict how to design polymer-coated nanorods to self-assemble end-to-end in a polymer film [48]. Such end-to-end alignment would enable tunable plasmon resonances between the nanorods for sensing applications [49]. In collaboration with Sandia Truman Fellow C. Ting, Frischknecht investigated transition pathways for patterned nanoparticles to cross polymersome membranes [50].

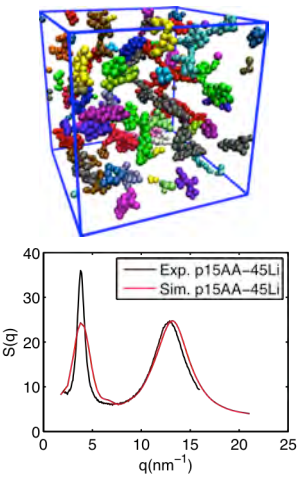

Figure 3. Top: MD snapshot of stringy ionic aggregates in an ionomer neutralized with lithium. Bottom: scattering profile from experiment (black) and MD simulation (red) for the same system. The first peak in S(q) is due to scattering from aggregates.

6.2.1.2 Structure on the Nanoscale

We have also made significant progress on understanding structure on the nanoscale in various soft materials. Here we highlight work on nanoscale morphology of ionic aggregates in ionomers and on the forces need to extend charged polymers such as ssDNA and hyaluronic acid.

Ionomers (polymers with a small fraction of charged ionic groups) form nanoscale ionic aggregates that strongly affect their mechanical and ion conduction properties [9]. Frischknecht and Stevens, in collaboration with CINT user K. Winey [51, 52], performed the first direct comparisons of scattering profiles obtained from atomistic MD simulations and from x-ray scattering in a series of precise poly-(ethylene-co-acrylic acid) copolymer and ionomer melts [53]. The simulations reveal ionic aggregates with a range of morphologies, from compact, isolated aggregates to branched, stringy aggregates to

branched, stringy aggregates that percolate through the simulation cell [54]. We found excellent agreement between the simulated and experimental scattering peak positions across all polymer types and aggregate morphologies (figure 3). Given the stringy aggregates found in many of the systems, we developed a new scattering model based on cylindrical aggregates. Surprisingly, we found that both spherical and cylindrical scattering models fit the scattering data for polymers with stringy aggregates equally well. This implies that the ionic aggregate morphology cannot be determined from the scattering data alone, but instead requires additional information such as that provided by simulation. This direct comparison of x-ray scattering data to the atomistic MD simulations is a substantive step toward providing a comprehensive, predictive model for ionomer morphology and provides new credibility to the presence of stringy, branched, and percolated ionic aggregates in precise ionomer melts.

The ionic aggregates have profound effects on the dynamics in ionomer melts. These dynamics can be probed experimentally by dielectric relaxation spectroscopy. As a first step toward connecting with those experiments and in consultation with CINT user J. Runt [55], we performed the first MD simulations on coarse-grained models of ionomer melts in an external electric field. We extracted the ionic mobilities and conductivities from the simulations, and found that ionomers with percolating ionic aggregates have the largest conductivities [56].

Grest and CINT user D. Perahia showed for the first time how the morphology and cluster size of ionic clusters depends on the strength of the electrostatic interactions [57]. Million-atom simulations of melts of randomly sulfonated polystyrene revealed how these changes in cluster morphology impact polymer mobility. For low dielectric media, the ionic groups form ladder-like clusters, but transform to more spherical clusters as the strength of the electrostatic interaction is reduced, resulting in higher mobility of the polymer, where controlling the mobility of the polymers is a key to the design of new classes of membranes for improved performance. They also carried out the first non-equilibrium molecular dynamics simulations of ionomers to determine how the mobility and shear viscosity of the polymer depends the counterion [58]. These simulations, in agreement with the experiments [59, 60], found that addition of only a small fraction of ionizable groups significantly increases the viscosity of the system. These results showed that slight changes in ionic content can serve as an excellent tool to tune desirable properties for membranes, opening the way to new smart materials.

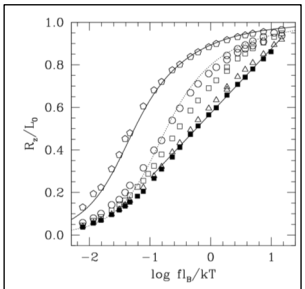

Figure 4. Semilog plot of normalized applied force vs. scaled extension for varying bending stiffness k_a for $k_a = 0$ (■), 1 (▲), 5 (□), 10 (○), and 50 (pentagon). Straight line is a fit to $k_a = 0$ at large extension. The curved lines are fits using the Marko-Siggia equation.

Stevens and CINT user O. Saleh [61-64] conducted MD and Monte Carlo simulations of force-extension curves for ssDNA, which is a flexible polyelectrolyte. The simulations reproduced the unexpected experimental finding of logarithmic scaling and found the unperturbed local chain structure is responsible for the logarithmic scaling. In anticipation of new experiments on other charged polymers, simulations have now treated varying the stiffness and the charge spacing. In varying the chain stiffness, the force-extension curves change from the logarithmic scaling of the flexible chain to match the Marko-Siggia [65] wormlike chain model of the semi-flexible chain (i.e. dsDNA). Our results, shown in Figure D, are further confirmation that the short length scale structure in the flexible chain is responsible for the logarithmic scaling.

6.2.2 Excitation and Transport in Nanostructured Systems

Both of the TSNP application areas for excitation and transport in nanostructured systems involve a dynamic research program combining methodological developments and applications to selected systems. User involvement has been extensive and includes both experimentalists, who come to the thrust for help interpreting their experiments; and theorists, who are involved in the development and application of our new methods.

6.2.2.1 Energy harvesting, non-adiabatic excitation, and quasiparticle dynamics

We have continued development of theoretical methods for describing large-scale electronic and vibrational dynamics beyond the ground state, and have applied them to experimentally relevant molecular systems

within the scope of CINT user program. The resulting Non-Adiabatic Excited State Molecular Dynamics (NA-ESMD) package became a world leading computational tool for modeling excited-state dynamics and radiationless relaxation in large molecular systems [23, 66]. With CINT users S. Fernandez-Alberti and A. Roitberg [67], Tretiak has applied this framework to model photoinduced processes in a complex dendritic system. Dendrimers, with their chemically controlled branched architectures, have enormous potential for achieving efficient light capture and transport. Here, in collaboration with ultrafast spectroscopist V. Kleiman, our calculations were able to explain experimental data and suggest new experiments in such complex molecular systems [68]. Our findings show that the electronic energy-transfer mechanism involves the ultrafast collapse of the photoexcited wave function due to non-adiabatic electronic transitions (see figure 5). This work provides a long-awaited consistent experiment–theoretical description of excited-state dynamics in organic conjugated dendrimers with atomistic resolution, a phenomenon expected to universally appear in a variety of synthetic conjugated materials. The knowledge gleaned from this study might help lay the groundwork for the development of improved organic photovoltaics and other solar energy conversion technologies.

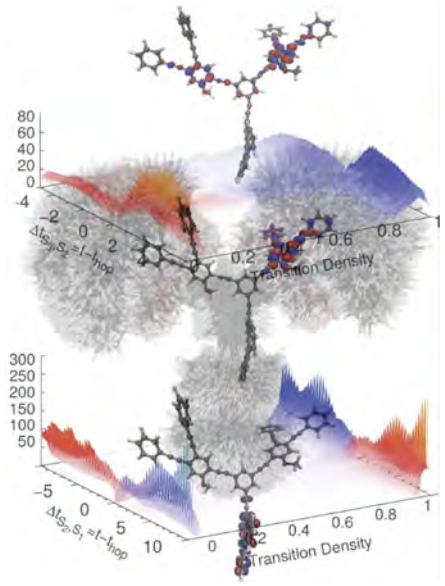

Figure 5. Illustration of the localization /delocalization mechanism as the main driver for the highly efficient and ultrafast transfer of energy in light harvesting dendrimers. (CINT highlight).

Among other CINT user projects, Tretiak and CINT user V. Chernyak [69] continued to extend ideas from the Exciton Scattering theory to establish a quite universal quasiparticle framework allowing treatment of complex electronic dynamics (e.g. exciton dissociation/recombination into charges, electron/spin dynamics, and phonon induced processes) in integrated nanosystems [70]. For example, in collaboration with CINT users O. Prezhdo and S. Kilina, our ab-initio molecular dynamics studies established the role of surface ligands in dephasing relaxation processes in quantum dots [71]. Our theoretical charge transport models in disordered electronic materials [72] were further guiding experiments to understand charge transfer dynamics in organic semiconductors and through biological pili filaments [73, 74], in collaboration with CINT users A. Zhugayevych, G. Bazan [75], and Martinez (SBCN). We have continued to support by electronic structure modeling CINT experimental efforts in the realm of chemically doped carbon nanotubes with Doorn and Htoon (NPON) [76]. Furthermore, our NA-ESMD modeling led experiments of Doorn's group on studying photophysical properties on novel cycloparaphenylene materials [77]. Finally in collaboration with CINT users C. Katan and J. Even [78], our quantum-chemical simulations helped experimental studies to achieve groundbreaking photovoltaic performance using new hybrid perovskite materials [79-81].

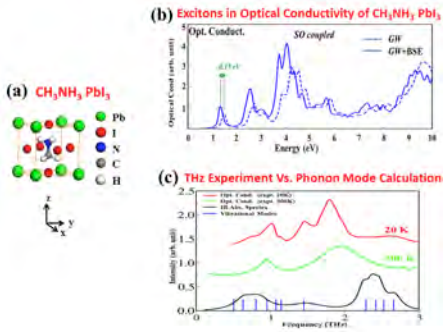

Figure 6. (a) Ionic relaxed crystal structure and Brillouin zone for the organometallic cubic perovskite $CH_3NH_3PbI_3$. (b) Presence of 150 meV exciton in the optical conductivity of cubic perovskite. (c) Theoretical and experimental phonon odes in the THz spectra of cubic solar cell perovskite.

In a parallel effort to understanding the perovskite solar cell materials, Zhu and CINT user Ahmed [82], have investigated the optical and vibrational properties of organometallic cubic perovskite $CH_3NH_3PbI_3$ (see figure 6a) using first-principles calculations [83]. For accurate theoretical description, we have gone beyond conventional density functional theory (DFT) and calculated optical conductivity using relativistic quasiparticle correction. Incorporating these many-body effects, we further solved Bethe-Salpeter equations (BSE) for excitons and found enhanced optical conductivity near the gap edge (see figure 6b). Due to the presence of organic methyl ammonium cations near the center of the perovskite cell, the system is sensitive to low-energy vibrational modes. We estimated the phonon modes of $CH_3NH_3PbI_3$ using a

small displacement approach and further calculated the infrared (IR) absorption spectra (see figure 6c). Qualitatively, our calculations of low-energy phonon frequencies are in good agreement with our terahertz measurements. Therefore, for both energy scales (around 1.5 eV and 0–20 meV), our calculations reveal the importance of many-body effects and their contributions to the desirable optical properties in the cubic organometallic perovskites system.

Although the above studies were performed for the cubic symmetry of the solar cell perovskite for computational simplicity, at room temperature (RT), the system was found to be in tetragonal phase while at low temperature, $CH_3NH_3PbI_3$ was in orthorhombic phase. With CINT user Chia, we have studied the temperature-dependent phonon modes of the organometallic lead iodide perovskite $CH_3NH_3PbI_3$ thin film across the terahertz (0.5–3 THz) and temperature (20–300 K) ranges [84]. These modes are related to the vibration of the Pb–b. These modes found that two phonon modes in the tetragonal phase at room temperature split into four modes in the low temperature orthorhombic phase. By use of the Lorentz model fitting, the critical behavior of this phase transition was analyzed. The carrier mobility values calculated from the low-temperature phonon mode frequencies, via two theoretical approaches, are found to agree reasonably with the experimental value ($\sim$2000 $cm^2\ V^{-1}\ s^{-1}$) from a previous time-resolved THz spectroscopy work. Thus, we have established a possible link between terahertz phonon modes and the transport properties of perovskite-based solar cells.

As system sizes increase from isolated molecules to the nanoscale, one important phenomenon is the development of bands of delocalized states with effectively continuum densities of states. In extended systems, a classical example of non-adiabatic dynamics is non-radiative carrier capture at a defect. In this process, a carrier in a delocalized band edge state makes a transition into a localized defect state with the resulting energy being absorbed by the emission of multiple phonons. With CINT user A. Wright [85], Modine has clarified the relationship between band edge states and defect states in DFT calculations [86]. This improved understanding has proven helpful both in interpreting the results of DFT calculations for defects [87, 88] and in developing a new approach to using DFT to calculate carrier capture rates [89]. The presence of a continuum of delocalized states can also enable the electronic subsystem to thermalize via electron-electron interactions on a time-scale where electron-ion interactions are still negligible. Working with CINT user Hatcher [90], Modine studied how this thermalization process and the resulting thermalized state is captured within the Time-Dependent Density Functional Theory (TDDFT) [91]. This represents an important first step toward applying TDDFT to problems such as ion-electron thermal equilibration and electronic heat transport.

6.2.2.3 Understanding Tunneling and Transport Experiments

Our computational study of tunneling experiments have focused on a series of physical systems, including conduction through graphene nanoribbons to distinguish between DNA bases well as to identify methylation or epigenetic signatures. DNA methylation plays a pivotal role in the genetic evolution of both embryonic and adult cells. Unusual methylation on CpG islands have been identified as one of the prime causes for silencing the tumor suppressant genes. Early detection of such methylation can diagnose the potentially harmful oncogenic evolution of cells and provide a promising guideline for cancer prevention. Our hypothesis is that electronic signatures of DNA acquired as a molecule translocating through a nanopore would be significantly different for methylated and non-methylated bases. With CINT user Ahmed [92], we calculated transport currents through a punctured graphene membrane while the cytosine and methylated cytosine translocate through the nanopore. We also calculated the transport properties for uracil and cyanocytosine for comparison [93]. Our first-principles calculations revealed significant distinct signatures in their spectrum for each molecular type,

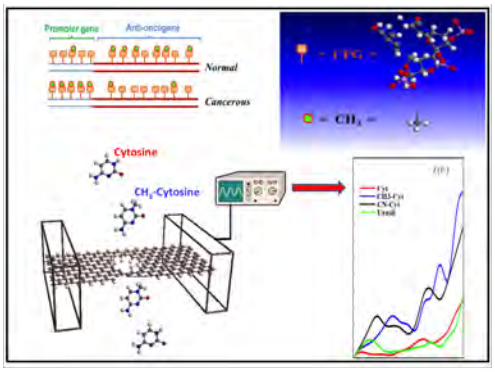

Figure 7. Schematic representation of DNA methylation. Excessive methylation in promoter gene is responsible for gene silencing of the antioncogenic part, which are often associated with different types of cancer.

particularly between methylated cytosine and its un-methylated form, as shown in figure 7.

As a viable method for fast and accurate DNA sequencing, we have also examined the mechanism of nanopore-based DNA sequencing using a voltage bias across a graphene nanoribbon. Using density function theory and a nonequilibrium Green's function approach, we determined the transmission spectra and current profile for adenine, guanine, cytosine, thymine, and uracil as a function of bias voltage in an energy minimized configuration. With CINT users Haraldsen and Ahmed, we provided a general methodology for the development of a three nanopore graphene-based device that can be used to distinguish between the various nucleobases for DNA/RNA sequencing [94]. From our analysis, we deduced that it is possible to use different transverse currents across a multinanopore device to differentiate between nucleobases using various voltages of 0.5, 1.3, and 1.6 V. Overall, our findings from this user project will help the nanopore design for improved DNA/RNA nucleobase sequencing and biomolecule identification techniques.

With CINT user Bonca [95], Trugman theoretically analyzed the dynamics of a photoexcited charge carrier coupled to quantum optical phonons in a nanowire. If the carrier excitation is sufficiently strong, the system relaxes after the primary energy redistribution towards a steady state. Then, the one-particle density matrix relevant for charge degrees of freedom along with the time-resolved optical conductivity takes the form of their thermal counterparts. The result indicates that steady states are (quasi)thermal and the temperature can be determined from the optical conductivity. Therefore, secondary relaxation processes observed in time-resolved ultrafast spectroscopy can be efficiently described by applying (quasi)thermal approaches, e.g., multi-temperature models [96].

6.2.3 Emergent Phenomena at Surfaces and Interfaces

To date, our TSNP work on interactions at surfaces and interfaces has been focused on understanding how these interactions induce emergent properties in complex oxide interfaces and the defect effects and on semiconductor surfaces and heterostructures with van der Waals materials.

6.2.3.1 Emergent Properties in Correlated Electron Heterostructures

Complex oxides are prototypical, strongly correlated electronic materials. They exhibit emergent phenomena such as ferroelectricity, magnetism, and superconductivity arising from competing interactions. When they are formed into heterostructures, the broken translational symmetry at the interfaces provides the basis for devices that take advantage of the unique opportunities for new emergent states. Although complexities arise due to orbital ordering and strain within the materials, investigations of the various couplings between different order parameters can provide information that is critical to the understanding of these heterostructures.

With CINT users Chia [97], Ahmed, Haraldsen [98], Jia (NEM), and Prasankumar (NPON), Zhu and Trugman have made significant progress in this area of research. The team has performed the DFT calculations on $BiFeO_3/La_{0.67}Sr_{0.33}MO_3$ (BFO/LSMO) superlattices and uncovered the dependence of the induced ferromagnetism at the BFO side of the interface on the band gap of bulk BFO [99] (see figure 8). We predicted that the exchange bias coupling ferromagnetic or antiferromagnetic between BFO and LSMO across the interface depends on the terminated atoms. This prediction was later confirmed by experiments [100].

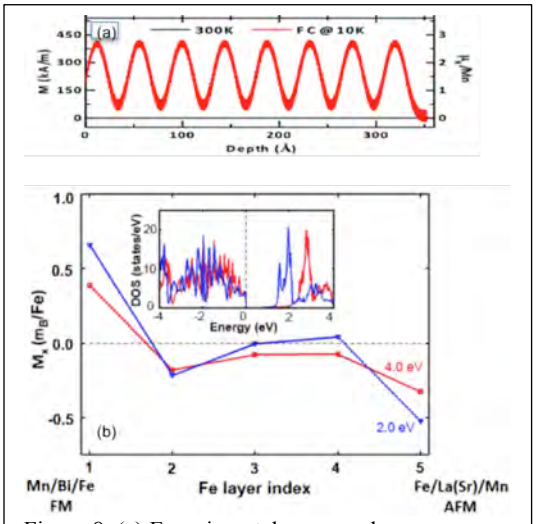

Figure 8. (a) Experimental measured magnetization in BFO/LSMO superlattice. (b) DFT-simulation of the ferromagnetic moment induction in the same material system.

We developed a new approach to the all-optical detection and control of the coupling between electric and magnetic order on an ultrafast timescale. This was achieved using time-resolved second-harmonic generation to study a ferroelectric/ferromagnetic oxide heterostructure, BSTO/LCMO (here BSTO stands

for $BaSrTiO_3$, and LCMO stands for $La_{0.7}Ca_{0.3}MnO_3$), an artificial multiferroic composite. In this heterostructure, the pump pulse photoexcites non-equilibrium quasiparticles in LCMO, applying stress on BSTO through magnetostriction. This then modifies the FE polarization through the piezoelectric effect, on a timescale much faster than laser-induced heat diffusion [101]. In addition, we also demonstrated an ultrafast polaronic transport in a BFO/LCMO heterostructure [102]. With CINT user Yarotski, we used femtosecond optical pump-probe spectroscopy to reveal the influence of charge and magnetic order on polaron dynamics and coherent acoustic phonon oscillations in the multiferroic material $LuFe_2O_4$. Multiferroics simultaneously possess spontaneous coupled electric and magnetic order. We observed a correlation between charge order and the amplitude of the acoustic phonon oscillations, due to photoinduced changes in the lattice constant that originate from photoexcited electrons [103]. These findings illustrate that the photoexcitation is a powerful tool to control the emergent order.

We also demonstrated a new approach for directly measuring the ultrafast energy transfer between electrons and magnons, enabling us to track spin dynamics in an antiferromagnet (AFM). In multiferroic $HoMnO_3$, optical photoexcitation creates hot electrons, after which changes in the spin order were probed with a THz pulse tuned to a magnon resonance. This revealed a photoinduced transparency, which builds up during several picoseconds as the spins heat up due to energy transfer from hot electrons via phonons. This spin-lattice thermalization time is about 10 times faster than that of typical ferromagnetic (FM) manganites. We qualitatively explain the fundamental differences in spin-lattice thermalization between FM and AFM systems and apply a Boltzmann equation model for treating AFMs. Our work gives new insight into spin-lattice thermalization in AFMs and demonstrates a new approach for directly monitoring the ultrafast dynamics of spin order in these systems [104].

CINT user Chia has also studied relaxation dynamics by performing ultrafast optical pump-probe measurement on a multiferroic-ferromagnetic $TbMnO_3$/LSMO bilayer [105]. We observed that the relaxation dynamics of the individual layers in the bilayer sample are the result of the interplay between the intrinsic magnetic order and the induced interfacial effect. Our data suggest the existence of induced ferromagnetic order in the $TbMnO_3$ layer and antiferromagnetic order in the LSMO layer. We also performed the DFT simulations on BFO/YBCO (YBCO stands for $YBi_2Cu_3O_7$) and predicted the emergence of ferromagnetic metallicity at the BFO side of the interface [106]. This discovery was then utilized to build an effective model to explain the ultrafast quasiparticle phenomena in the same system [107]. We also studied the electronic, magnetic, and optical properties of double perovskite Bi_2FeMnO_6 (BFMO), which can be regarded as an extreme limit of interfacial engineering, and we resolved for the first time the noticeable size of ferromagnetic moment from magnetization measurements [108]. In addition, we introduced a model with Fe/Mn chemical disorder in the surface layers of BFMO to explain the weak ferromagnetic signal obtained in XMCD [109].

The high research output in this area has benefited from a concerted effort among TSNP/NPON/NEM thrusts and multiple users.

6.2.3.2 Semiconducting Compound Surface and Interface Structure

Working with CINT user groups Millunchick and Van de Ven [110-112], Modine has continued to develop an approach combining DFT, the cluster expansion method, and Monte-Carlo (DFT/CE/MC) to model thermodynamic and kinetic behavior with DFT accuracy while accounting systematically for compositional and structural disorder [113, 114]. This approach, which was initially applied to semiconductor surfaces at CINT, has more recently been an important component of CINT user research targeting bulk properties and defect behavior in semiconductor alloys. Modine also worked with CINT user Noda [115] to study the ZnO/Cu_2O interface and with the group of CINT user Krishna [116, 117] to study the InAs/GaSb interface and the properties of InAs/GaSb superlattices [118].

With CINT user Ahmed, Modine and Zhu performed DFT calculations for a bi-layered heterostructure combining a graphene layer with a MoS_2 layer with and without intercalated Li atoms [119]. Our calculations demonstrated the importance of the van der Waals interaction, which is crucial for forming stable bonding between the layers. Our DFT calculation correctly reproduced the linear dispersion, or Dirac cone, feature at the Fermi energy for the isolated graphene monolayer and the band gap for the MoS_2 monolayer. For the combined graphene/MoS_2 bi-layer, we observed interesting electronic structure

and density of states characteristics near the Fermi energy, showing both the gap-like features of the MoS_2 layer and in-gap states with linear dispersion contributed mostly by the graphene layer. We also found that intercalating Li ions in between the layers of the graphene/MoS_2 heterostructure enhances the binding energy through orbital hybridizations between cations (Li adatoms) and anions (graphene and MoS_2 monolayers).

With CINT user Ahmed and Yoo (NEM), we also studied the charge transfer effect on a series of semiconductor hetrostructures. Using DFT simulations, we observed significant charge transfer from bulk Ge (semiconducting) onto MoS_2 single layer (insulating) turning the combined system into metallic. Such findings have deep impacts on developing the next generation n-p semiconducting junction [120]. A similar phenomenon was also observed in single layer graphene grown on the top of bulk ZnO substrate [121].

6.3 Proposed Work

6.3.1 Hierarchical Structure and Dynamics in Soft Matter

Future work within this science direction will include an increased focus on charged and magnetic polymers. Charged nanoparticle systems can form hierarchical structures, which can be modified by rather easily adjustable conditions (e.g. salt concentration). Having added dipolar interactions in our MD code LAMMPS, CINT users will be able to study the magnetic hierarchical nanoparticle systems.

6.3.1.1 Nanoparticle Structure and Assembly

Inorganic nanoparticles have tunable optical and electronic properties [122]. Control of their assembly could therefore lead to a variety of interesting material properties [123]. One relatively unexplored area for theory and simulation of NP assembly is the assembly of charged NP and the dependence of the assembly on the electrolyte environment in solution. We recently began to model the interactions between charged NPs and have developed an understanding of the parameter space for attractive interactions between like-charged NPs [34]. One new focus will be studying ensembles of many charged NPs to develop an understanding of how to manipulate the assemblies to control material properties [124-128]. Charged coatings are one means to solvate NPs in water. We propose to carry out further simulations to develop a basic foundation of knowledge on the assembly of charged NPs under varying salt conditions and varying levels of charging of the NPs. We will then pursue more complicated systems that possess a hierarchy of structure and properties. One example is a mixture of charged NPs with distinct cores A and B, which could be ordered in the liquid solution such that near neighbors of A are B particles and vice versa. With the appropriate interaction between the cores, some new material capability could be created because the distinct cores can be sufficiently close to alter one other's properties.

One important application of NPs is in sensing applications ranging from single molecule microscopy to a low-cost, portable diagnostic device [129]. For these applications, the NP coating is particularly critical with respect to ensuring high selectivity and sensitivity for detection. For example, imperfect polymer coatings can result in exposed surfaces that are non-specifically adsorptive, resulting in decreased signal-to-noise levels and increased false positives. Fully-atomistic classical MD simulations coupled with experiments by Bachand (SBCN) will be carried out to understand the organization of polymer coatings on NPs for carrying and exposing reactive-probe end groups and relate their organization to use as a biomolecular probes. We will leverage our previous modeling [29, 130] that has shown that certain coatings on small particles are susceptible to coating asymmetry and patchiness that would lead to loss of selectivity. However, that work was focused on smaller NPs ($\leq$ 8 nm diameter), nonpolar chains and homogeneous coating chain lengths. Biomolecular probes will require significant extension of these parameters to include NP diameters from 20–40 nm, mixed ligand chain lengths, and allow for chain migration on the NP surface. We will systematically study the role of NP size and shape, and composition, length, and coverage on the organization of the ligands coating and correlate this information with experimental data regarding the efficacy of antibody conjugation and the selectivity and sensitivity of the final NP probe. Gold NPs/nano-rods with mixed coatings of thiol-terminated polyethylene glycol (PEG) with different chain lengths will be used as the model system.

We recently developed the capability to treat dipolar interactions in the LAMMPS MD code [131]. This new capability will allow CINT users to model how the magnetic interactions between NPs can be used to

direct NP assembly in an applied field. Initially simulations to determine the phase diagram of dipolar NPs as a function of the NP dipole, concentration and applied field strength will be carried. Of particular interest is to determine the conditions for assembly of NPs into strings and crystals (e.g. body centered tetragonal). As imaging and measuring of these NP structures is difficult and tedious, the simulations can greatly reduce the parameter space that must be measured experimentally. Once the phase diagram of the magnetic NPs in solution is known, how the dipolar interactions can be used to construct nanocomposites in polymer matrices and examine how using a field can manipulate the positioning of the NPs will be investigated. The simulations will be validated by comparing to the experimental results of Huber (SBCN).

6.3.1.2 Structure of the Nanoscale

As introduced above, in collaboration with several CINT users, we have developed an ongoing research program into the consequences of the nanoscale structure and dynamics of ionic aggregates on the properties of ionomers. The addition of even a small number of ionizable groups impacts both the dynamics of the melts and their ability to transport ions and solvents. We have focused on two material systems that have been extensively studied experimentally: a set of precise ionomers with exact spacing between ionic groups along a polyethylene backbone and randomly sulfonated polystyrene (PSS). Of particular interest are the effects of varying counterion size and valency and ionic group on chain mobility and the response of these ionomers to external fields such as shear and electric fields.

In related ionomers research, we are interested in ion transport and understanding the connection between structure and improved conductivity. We already found that differences in polymer architecture affect the aggregate structure substantially, i.e. percolated vs. isolated aggregates [132]. We will investigate multiple facets of the nanoscale structure's connection to dynamics in both precise ionomers and PSS. We are working closely with experimental groups to compare our simulation data with their experimental data. For the precise ionomers, we will compare the dynamics obtained from atomistic MD simulations with quasielastic neutron scattering to further understand how ionic aggregates modify chain and ion dynamics. We will extend our coarse-grained model of generic ionomers to include the dipole moment of the backbone, using the new dipole capability in LAMMPS, so that we can have a full comparison to dielectric relaxation spectroscopy experiments that probe both chain and ion dynamics on larger length and time scales. We will extend our treatment of precise ionomers to additional ionic groups, particularly sulfones and sulfates that are being studied experimentally. We will also investigate how the ionic aggregates affect the unique mechanical properties of ionomers.

We are also examining the crystallite structure formed below T_g in the precise ionomers. By comparing atomistic MD simulations to x-ray data of user Winey, we will determine the location of the ionic groups in the crystallites. Preliminary results suggest that the ionic groups are at the surfaces of the crystallites. This opens the question of whether ionic transport is faster at the crystallite surface or at an ordered structure than in a more disordered system. Related to this is recent work on carboxyl terminated self-assembled monolayers (SAMs), which found good conductivity between SAMs [133]. We intend to directly simulate the SAM systems to examine the ion transport in the detail that simulation allows and to use SAM systems to investigate other chemistries. We expect this will give new insight into ion transport mechanisms.

Lightly sulfonated polystyrene oligomers, at molecular weights significantly below the entanglement length of the polymer, are known experimentally to be highly viscous and that diffusion is significantly hindered in comparison with non-sulfonated polystyrene with an identical chain length [59, 60]. This large change in the dynamic response is due to formation of ionic clusters that act as physical cross-linkers. With CINT user Perahia, we will correlate structure and size of the ionic clusters in PSS melts with different mono and divalent counterions with the dynamics on multiple length and time scales extracted from measurements of the dynamic structure factor and shear rheology. Being able to probe computationally long times commensurate with the actual segmental dynamics time-scales in ionomers, now possible with new computational tools, will provides a new fundamental insight into the factors that impact the dynamics of ionic polymers.

In addition to developing an understanding of how nanoscale ionic aggregates affect bulk properties of ionomers, we propose to investigate these aggregates near interfaces. Both mechanical properties and ion transport are strongly affected by the detailed structure at either self-assembled interfaces such as those that

form in block copolymers, or at polymer-solid interfaces such as electrolyte-electrode interfaces. Understanding of the nanoscale structure at interfaces will further advance our ability to design ionomers for desired properties and integration into devices in the future.

6.3.2 Excitation and Transport in Nanostructured Systems

A growing effort within this science direction is supporting our vision of hybrid material interaction for energy/information generation and manipulation in integrated structures.

6.3.2.1 Energy harvesting, non-adiabatic excitation, and quasiparticle dynamics

Tretiak, in collaboration with CINT users, will continue to develop a theoretical framework for treatment of non-adiabatic electron-phonon dynamics in extended molecular systems [23, 134]. A path forward highlights several key groundbreaking developments to be implemented our NA-ESMD suite. i) Photochemistry and bond-breaking [135, 136]: Decomposition of the system into sub fragments requires "an open shell" framework (each electron occupies its own orbital). Formulation of non-adiabatic excited state dynamics for such processes remains unsolved problem worldwide. Our recent work proposed theoretical description, which will be algorithmically refined and implemented in this project. ii) Extended Lagrangian dynamics and O(N) scaling: This framework has been developed for ground state simulations. Formulation for excited state dynamics will allow dramatic expansion of range of treatable systems by going from 10^2 to 10^4 atom system size. iii) Quantum control and coherence: Existing practical methods for non-adiabatic dynamics simulations (Ehrenfest and surface hopping) fail to describe evolution of interferences and coherences in electronic systems, which are very important in any light-driven dynamics. Recently we have developed a new theoretical framework addressing this long-standing problem [137-140]. Numerical implementation of this method relying on the graphs will allow simulations of coherent control optical experiments without an increase in numerical cost. iv) "Hamiltonian on demand": Our NA-ESMD code currently uses standard semiempirical Hamiltonian models for quantum simulations. Here we will implement on-the-fly fitting of the reduced Hamiltonian (tight-binding DFT, DFTB, or semiempirics) for a given material/molecular family relying on high quality quantum-chemical simulations. v) "Quantum-classical interface": Non-equilibrium quantum dynamics is frequently spatially localized but is strongly influenced by a surrounding solvent, solid-state matrix, etc. This permits introduction of so-called hybrid quantum mechanics/molecular mechanics (QM/MM) approach by interfacing quantum and classical MD regions. Our recently developed state-specific solvation models [141-143], in which dielectric environment responds to specific excited states, will be implemented in a full QM/MM frame. These theoretical and algorithmic advances altogether present an unprecedented integrate framework revolutionizing first-principle-based molecular dynamics beyond the ground state. Their computational implementation will be taking a full advantage of LANL high performance computing in terms of large-scale data processing, parallelism, and portability to future-generation computing architectures. At CINT we have exceptional access to experimental data (such as high quality spectroscopic probes) for validation of every theory component. Furthermore, any further development can immediately provide a substantial boost to a number of already running programs and collaborations at CINT user program. New developments will compose computationally tractable approach applicable to a full spectrum of systems and phenomena. Their applications include, but are not limited to, vibronic dynamics in dendrimeric macromolecules and carbon nanotubes, evolution of photoexcitation and charge separation in conjugated polymers, and energy pathways in biological light harvesting systems. Our detailed theoretical modeling will facilitate experimental realization of these nanosystems and verification of our predictions in collaboration with NPON and NEM thrusts scientists.

The design of devices capable of controlling the light-matter interaction at the nanoscale has been a subject of intense interest. Tailored metallic nanostructures are ideal candidates for this purpose with their ability to focus and trap optical energy into subwavelength regions in space. These systems can thus be strongly coupled to other photonic objects like quantum emitters. To understand the physics underlying the internal interaction in these hybrid systems, the quantum features play an important role. We plan to develop a fully quantum mechanical approach to describe the coupling between plasmonic and excitonic degrees of freedom. From the proposed research, we will develop new capability for new optical functionality arising from these interactions.

6.3.2.2 Understanding Tunneling and Transport Experiments

In this section, we will focus more on transport through nanoscale structures: quantum dots, quantum impurities, quantum wires. These studies are well aligned with the CINT's new research direction on quantum information.

We will build upon our existing expertise on the quantum impurity/spin coupled with normal metallic contacts to develop understanding of the quantum coherence and transport when these nanoscale systems are coupled with unconventional environments like the surfaces of topological insulators. The understanding requires a careful characterization of interfacial interaction between nanoscale components and these underlying hosting materials. Our efforts will be developing a predictive capability for the relation between interfacial structure and functionality. In this area, a joint experimental and theoretical study of the optical and Terahertz spectroscopy of Weyl semimetals and their associated topological chiral anomaly will be carried out. We are also planning ultrafast studies of topological insulator Bi_2Se_3. New user projects will be established in this area with joint efforts in NEM and NPON thrusts.

In a new project, CINT user Myers [144] and TSNP scientist Modine established that tunneling between interfaces and defects can have a dramatic effect on the electrical behavior of defect-containing heterojunction devices. By tunneling across an interface, carriers can be captured from states that are close in energy to a localized defect state, and this can increase the rate of non-radiative carrier capture—and hence the rate of carrier recombination, by several orders of magnitude. We have developed an initial model that incorporates both the tunneling and non-radiative carrier capture processes, and the results of this model agree well with experiments on radiation damaged heterojunction bipolar transistors. This is a particularly exciting area of research because it bridges across three TSNP themes: tunneling, interfaces, and non-adiabatic dynamics. In future work, we will refine and extend our model and consider a wide variety device geometries (e.g. defects within barriers or superlattices).

With CINT user Bonca, we plan to theoretically investigate the dynamics of an electron in a nanowire coupled to phonons and driven by an AC THz/IR pulse. The electron and phonons will be treated fully quantum mechanically using a numerically exact algorithm we developed. Preliminary results show coherent oscillations and an expanding range of correlations between the electron and phonon excitations.

6.3.3 Emergent Phenomena at Surfaces and Interfaces

We will now discuss our ongoing work in the areas of emergent phenomena, including new opportunities for experimental collaboration within CINT, and semiconductor interfaces.

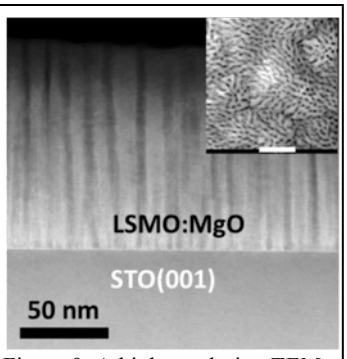

Figure 9. A high-resolution TEM image of a nanocomposite $MgO:La_{0.7}Sr_{0.3}MnO_3$ grown on $SrTiO_3$ substrate.

6.3.3.1 Emergent Properties in Strongly Correlated Heterostructures

Trugman and Zhu will continue working with the NEMS thrust and CINT users on the emergent phenomena arising in the complex oxides and the interfaces between these materials with competing orders, as well as those between complex oxides and other materials with new states of matter. We will study the interplay between competing orders at the interface from the constituent materials, and understand the functionality response. Building upon our past success in the study of magnetic properties at the interface of planer heterostructures, we will expand to study the interfacial effects on the emergent phenomena in pillar and particular structures. One example of pillar-type interface structure is shown in figure 9. There it has been found that the ferromagnetism is very sensitive to the pillar concentration of MgO but not ZnO. This different response has yet to be understood. We are particularly interested in the working principles for an optimal figure of merit, for example the magnetoelectric effects. We will continue to apply the DFT theory to study both structure and function relation in these interesting heterostructures. We will calculate not only the magnetic moment but also the ferroelectric order in nanocomposites with DFT in planer heterostructures. We will also develop a tight-binding model capability to study the interplay between magnetic and ferroelectric orders. The low-energy tight-binding model will be informed with the material's specific information obtained with DFT band structure simulations. The tight-binding model will enable the simulations at the mesoscopic scale and is necessary to model the

electronic, magnetic, ferroelectric response to the microstructures, defects, and impurities at the interface of nanocomposites. It will also provide a framework to include the matter-radiation interaction for the ultrafast control. There an AC field with varying strength and frequency can tune the spin-spin interaction and electron hopping [145] and we will investigate enhanced ultrafast magnetoelectric coupling in a FM-manganite/FE-oxide heterostructures. The research development in this area will be fully aligned with the new DOE-BES initiative in mesoscale science.

6.3.3.2 Semiconducting Compound Surface and Interface Structure

We will further develop our DFT/CE/MC approach to DFT-based computational statistical mechanics and continue to apply it to determine bulk, surface, interface, and defect properties for systems with compositional and structural disorder. One important development will be the implementation of a recently developed approach to incorporating the long-ranged electrostatic interactions between charged ions. The proper treatment of these interactions is particularly important for accurate modeling of materials involving heterovalent substitution (e.g., substitution of In for Cu in the $Cu(In_{1-x}Ga_x)Se_2$ alloy) or intercalation of a charged species (e.g., Li^+ motion in a solid electrolyte). Capturing these long-range interactions is also essential to understanding the compensation of charged surfaces and interfaces by structural reconstruction or defects. We will also continue our work investigating the interfaces and interactions between 2-D materials such as graphene and MoS_2, where a huge variety of structures can be constructed from a few basic building blocks by varying the stacking sequence and intercalating different atoms or small molecules between the layers.

6.3.3.3 Model and Methods Development

A goal that unifies the efforts within this science direction is the development of theoretical tools to bridge between the nanoscale/atomic and the macroscopic scale, which sits at the core of hybrid structures. In addition, the capability to describe the phenomena at atto and femtosecond intrinsic time scales of electronic and vibrational dynamics to the pico and nanosecond time scales associated with transport and energy redistribution in nanostructures should also be enabled in the tools. Combined with the subatomic spatial resolution of modern theoretical methods, this major capability development will allow us to understand how the dynamical properties of macroscale systems arise from the behavior of the system at extremely various length and time scales. TSNP scientists Modine, Tretiak, Trugman, and Zhu, will work together to address this challenging area and in particular ramp up the efforts on the calculations of electronic, magnetic, and optical properties in complex oxides and other functional materials. These focused efforts will significantly enhance our capability to address the challenge in the research at mesoscale. Through the ongoing user projects, we will develop new computational package dedicated to explore the structure and function relations first in transition-metal oxide nanocomposites and later on extended to other functional materials. In particular, we will also leverage our institutional expertise to construct *ab-initio* informed low-energy tight-binding based models into this new package for multiscale modeling of emergent phenomena.

To conclude, the TSNP thrust represents a well-balanced set of theory and simulation skills that enable us to address the diverse needs of CINT users. The complementary skills of Los Alamos and Sandia allows us to cover a wide range of topics spanning hard and soft systems and to model molecular, electronic, optical, thermal, mechanical, and magnetic properties of integrated nanoscale materials and systems. Despite this diversity, we are able to maintain strong areas of focused research. The TSNP thrust features thrust-centric activities in parallel with experimentally driven research. Many of our capability development efforts are examples of thrust-centric work. Numerous examples of intra-thrust and inter-thrust collaborations have been discussed above. CINT users, both experimentalists and theorists, contribute to all aspects of the work within the thrust. The development of new capabilities will not only directly support the CINT strategic plan but also provide new opportunities to enhance focused collaboration between TSNP scientists, CINT experimental thrusts, and users.

7.0 Publications

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7.2 Publications from Previous Support

	TSNP Publication Count			
NSRC High Impact Journals	**2013**	**2014**	**2015**	**Total**
ACS Nano	0	2	2	**4**
Advanced Functional Materials	0	0	0	**0**
Advanced Materials	0	1	1	**2**
Angewandte Chemie International Edition	0	0	0	**0**
Applied Physics Letters	1	3	2	**6**
Chemistry of Materials	0	0	0	**0**
Journal of the American Chemical Society	1	1	1	**3**
Nano Letters	0	2	0	**2**
Nanoscale	0	1	1	**2**
Nature	0	0	0	**0**
Nature Chemistry	0	0	0	**0**
Nature Communications	0	1	0	**1**
Nature Materials	0	0	0	**0**
Nature Nanotechnology	0	0	0	**0**
Nature Photonics	0	0	0	**0**
Nature Physics	0	0	0	**0**
Physical Review Letters	4	5	1	**10**
Proceedings of the National Academy of Sciences USA	0	0	0	**0**
Science	0	0	1	**1**
Small	0	0	0	**0**
TOTAL:	6	16	9	**31**

TSNP

2013 Publication total: 41
CINT science: 16
CINT user science (internal): 5
CINT user science (external):20

2014 Publication total: 53
CINT science: 18
CINT user science (internal): 4
CINT user science (external): 31

2015 Publication total: 49
CINT science: 8
CINT user science (internal): 15
CINT user science (external): 26

Note: CINT Scientist authors are indicated in red; CINT User authors are indicated in green (external) and orange (internal).

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8.0 Biographical Sketches

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Distinguished Member of Technical Staff, Sandia National Laboratories, 1998-present
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Editor, Physical Review E, 2002-2012
Adjunct Professor, Department of Chemistry, Clemson University, 2009-
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High Strength, Molecularly Thin Nanoparticle Membranes, K. M. Salerno, J. M. D. Lane, D. S. Bolintineanu, and G. S. Grest, Phys. Rev. Lett. 113, 258301 (2014).
Ligand Structure and Mechanical Properties of Single-Nanoparticle Thick Membranes, K. M. Salerno, D. S. Bolintineanu, J. M. D. Lane, and G. S. Grest, Phys. Rev. E 91, 062403 (2015).
Clustering Morphology in Ionic Polymers: Molecular Dynamics Simulations, A. Agrawal, D. Perahia, and G. S. Grest, Phys. Rev. E 92, 022601 (2015).

Synergistic Activities
Awards:
Chaim Weizmann Postdoctorate Fellowship, 1977 - 1978
Alfred P. Sloan Foundation Fellowship, 1981
Best Paper in Acta Metallurgica, 1985
Fellow - American Physical Society, 1989

Sandia Computational Science Prize, 1st Place, 2001
Alexander Humboldt Senior Research Fellow, 2002
Award for Excellence, Laboratory Research and Development, 2006
American Physical Society Aneesur Rahman Prize in Computational Physics, 2008
Member of the National Academy of Engineering, 2008
American Physical Society Polymer Physics Prize, 2011
Hall of Distinction, Louisiana State University, College of Science, 2013
Publications: 12 reviews, 430 journal articles
Professional Society Offices: Member-at-Large - Executive Committee of the Division of Condensed Matter Physics, American Physical Society, 1992-1995
Advisory Board:
Divisional Associate Editor, Physical Review Letters, 1994-2000
Institute for Theoretical Physics, University of California, Santa Barbara, 2001-2003
Organizer, Workshop on Theory and Simulation of Nano Scale Materials, Center for Integrated Nanotechnologies, Sandia National Laboratories, 2010
Organizer, Joint NSRC Workshop on Nanoparticles, Center for Nanoscale Materials, Argonne National Laboratory, 2012
Organizer, 2014 Division of Polymer Physics, American Physical Society, Short Course on "Multiscale Computational Approaches for Simulating Polymers from Atomistic to Mesoscale"

Collaborators (last 48 months, outside of Sandia): Shengfeng Cheng (Virginia Tech), Alexander Y. Grosberg (New York University), Ting Ge (University of North Carolina), William T. Heller (ORNL), Ahmed Ismail (University of West Virginia), Heinrich Jaeger (University of Chicago), Kurt Kremer (Max Planck Institute, Germany), Sanat Kumar (Columbia University), Christian Lorenz (King's College, London), Athanassios Panagiotopoulos (Princeton), Dvora Perahia (Clemson University), Mark O. Robbins (Johns Hopkins University), Michael Rubinstein (University of North Carolina), Kenneth S. Schweizer (University of Illinois), Leo Silbert (University of Southern Illinois), Mesfin Tsige (University of Akron), Pieter in 't Veld (BASF, Germany), Carl L. Willis (Kraton LLC).

Graduate and Postdoctoral Advisors: A. K. Rajagopal, Naval Research Laboratory, Washington, D. C. (Ph.D. Advisor); E. Abrahams and M. J. Stephen, Department of Physics, Rutgers University (Post-Doctoral Advisors, 1974-1977); M. H. Cohen, Department of Physics, The University of Chicago (Post-Doctoral Advisor, 1977-1978)

Thesis Advisor and Postgraduate-Scholar Sponsor: (over the last 5 years)
Students: Sabina Maskey, Dipak Aryal, and Sidath Wijesinghe (Clemson University)
Postdocs: Anupriya Agrawal (Clemson University), Dan S. Bolintineanu (Sandia), Shengfeng Cheng (Virginia Tech), Flint Pierce (Sandia), Brandon Peters (Sandia) and K. Michael Salerno (Sandia).

Total: 3 students, 6 postdocs

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Education:

Undergraduate:	Department of Physics, Nanjing University, July 1990, B.Sc.
Graduate:	Department of Physics, Nanjing University, July 1993, M.Sc.
	Department of Physics, University of Hong Kong, Dec. 1997, Ph.D.

Professional Experience:

October 2004 – present	Staff member, Theoretical Division, LANL
August 2012 – present	Partner Science Leader, CINT, LANL/SNL
July 1, 2012 – June 30, 2017	Adjunct full professor, Rice University
February 2013 – August 2017	Adjunct full professor, University of Houston
July 2001 – September 2004	Director-funded postdoctoral fellow, LANL
Sep. 2002 -- Dec. 2002	Visiting scientist, Rice University
Sept. 2000 -- July 2001	Research assistant professor, University of Houston
June 1997 -- August 2000	Postdoctoral fellow, University of Houston

Publications:

Towfiq Ahmed, N. A. Modine, and Jian-Xin Zhu, Bonding between graphene and MoS_2 monolayers without and with Li intercalation, Appl. Phys. Lett. 107, 043903 (2015).

Jian-Xin Zhu, R. C. Albers, K. Haule, and J. M. Wills, First-principles study of the Kondo physics of a single Pu impurity in a Th host, Phys. Rev. B 91, 165126 (2015)

Towfiq Ahmed, C. La-O-Vorakiat, T. Salim, Y. M. Lam, Elbert E. M. Chia, and Jian-Xin Zhu, Optical properties of organometallic perovskite: An ab initio study using relativistic GW correction and Bethe-Salpeter equation Europhys. Lett. 108, 67015 (2014).

Jian-Xin Zhu, Xiao-Dong Wen, J. T. Haraldsen, Mi He, C. Panagopoulos, and Elbert E. M. Chia, Induced ferromagnetism at $BiFeO_3/YBa_2Cu_3O_7$ interfaces, Sci. Rep. 4, 5368 (2014).

S. Singh, J. T. Haraldsen, J. Xiong, E. M. Choi, P. Lu, D. Yi, X.-D. Wen, J. Liu, H. Wang, Z. Bi, P. Yu, M. R. Fitzsimmons, J. L. MacManus-Driscoll, R. Ramesh, A. V. Balatsky, Jian-Xin Zhu, and Q. X. Jia, Induced magnetization in $La_{0.7}Sr_{0.3}MnO_3/BiFeO_3$ superlattices, Phys. Rev. Lett. 113, 047204 (2014)

Jie Ren and Jian-Xin Zhu, Anomalous energy transport across topological insulator superconductor junctions, Phys. Rev. B 87, 165121 (2013)

Jian-Xin Zhu, Rong Yu, A. V. Balatsky, and Q. Si, Local electronic structure of a single nonmagnetic impurity as a test of the pairing symmetry of electrons in (K,Tl)FexSe2 superconductors, Phys. Rev. Lett. 107, 167002 (2011).

A. V. Balatsky, I. Vekhter, and Jian-Xin Zhu, Impurity-induced states in conventional and unconventional superconductors, Rev. Mod. Phys. 78, 373 (2006).

Jian-Xin Zhu, K. H. Ahn, Z. Nussinov, T. Lookman, A. V. Balatsky, and A. R. Bishop, Elasticity-Driven Nanoscale Electronic Structure in Superconductors, Phys. Rev. Lett. 91, 057004 (2003).

Jian-Xin Zhu, Ivar Martin, and A. R. Bishop, Spin and Charge Order around Vortices and Impurities in High-Tc Superconductors, Phys. Rev. Lett. 89, 067003 (2002).

Synergistic activities:

Principal organizer, The CNLS 35th Annual Conference on Electronic Structure Approaches and Applications to Quantum Matter, Santa Fe (2015)

Co-organizer, CECAM Workshop in Gutzwiller Wave Functions and Related Methods, Valence, France (2014)

Reviewer of Natural Science Foundation (NSF) and Department of Energy (DOE)

Referee of Physical Review and Physical Review Letters, Journal of Physics: Condensed Matter, Physics

Letters A, Europhysics Letters, New Journal of Physics, Physica E, and International Journal of Modern Physics B.
Member of the American Physical Society
Member of the Materials Research Society
2013-2014: Member, the LDRD-ER-EPM Committee
2012-2013: Member, the LDRD-ER-EPM Committee
2011-2012: Member, the LDRD-ER-DIM Committee
2010-2011: Member, the LDRD-ER-EPM Committee

Research experience & accomplishments:
Expertise in strongly correlated electron materials, impurity problem in strongly correlated electron systems, quantum phase transition in heavy fermion systems, structure and properties in nanoscale electronic systems. Experienced in theoretical analysis in STM and ARPES experiments. Authored and co-authored more than 220 peer-reviewed publications.

Honors:
Achievement Award, Los Alamos National Laboratory (2015)
Postdoctoral Distinguished Performance Award, Los Alamos National Laboratory (2003)
Li Ka-Shing Prize for the Best Ph.D. Thesis, the University of Hong Kong (1997)

Collaborators: J. Haraldsen (Univ. of Northen Florida); J. C. Davis (Cornell); Matthew Jones (Univ. of Buffalo); Q. Si (Rice Univ.); R. Bulla (Augsberg Univ.); J.-P. Julien (Institut Neel CNRS); C. S. Ting (Univ. of Houston); Elbert Chia (Nanyang Technology Univ.); Jianhui Dai (Hangzhou Normal University); G. Kotliar (Rutgers Univ.); K. Haule (Rutgers Univ.); H. Q. Yuan (Zhejiang University); Rong Yu (China Renming University); Zhi-Xun Shen (Stanford); K. Bassler (Univ. of Houston); J. Fransson (Uppsala)

Graduate and Postdoctoral Advisors: Z. D. Wang (University of Hong Kong, Ph.D. Advisor); C. S. Ting (University of Houston, Postdoctoral Advisor); A. V. Balatsky (Los Alamos National Laboratory, Postdoctoral Advisor)

Thesis Advisor and postgraduate Scholar - Sponsor: Postdoc scholars sponsored – Towfiq Ahmed, Cheng-Ching Joseph Wang, Jie Ren, Lijun Zhu, Haitao Quan, and Jianmin Tao; Graduate students mentored – Yuan-Yen Tai, Robert Beaird, Xiang Hu, and P. M. R. Brydon.

Students/postdocs mentored in the last 5 years: 7 postdocs, 2 students

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Education
Ph.D. University of California, Santa Barbara, Physics, September 1998
B.A. Pomona College, Physics and Mathematics (summa cum laude), May 1992

Professional Experience:
Principal Member of Technical Staff, Sandia National Laboratories, Oct. 2006 – present
Senior Member of Technical Staff, Sandia National Laboratories, May 2003 – Oct. 2006
Postdoctoral Appointee, Sandia National Laboratories, Oct. 2000 – May 2003
Postdoctoral Fellow, ExxonMobil Research and Engineering Co., Oct. 1998 – Oct. 2000
NSF Fellow, Graduate Student Researcher, Doctoral Scholar Fellow, and UC President's Dissertation Year Fellow, Department of Physics, University of California, Santa Barbara, Sept. 1992-Sept. 1998

Publications
C. L. Ting, R. J. Composto, and A. L. Frischknecht, Orientational Control of Polymer Grafted Nanorods, Macromolecules 49**,** 1111–1119 (2016).
C. F. Buitrago, D. S. Bolintineanu, M. E. Seitz, K. L. Opper, K. B. Wagener, M. J. Stevens, A. L. Frischknecht, and K. I. Winey, Direct Comparisons of X-ray Scattering and Atomistic Molecular Dynamics Simulations for Precise Acid Copolymers and Ionomers, Macromolecules 48**,** 1210–1220 (2015).
C. L. Ting, M. J. Stevens, and A. L. Frischknecht, Structure and Dynamics of Coarse-Grained Ionomer Melts in an External Electric Field. Macromolecules 48**,** 809–818 (2015).
C. A. Lueth, D. S. Bolintineanu, M. J. Stevens, and A. L. Frischknecht, Hyrdogen-bonded aggregates in precise acid copolymers, J. Chem. Phys. 140**,** 054902 (2014).
A. L. Frischknecht, M. J. A. Hore, J. Ford, and R. J. Composto, Dispersion of Polymer-Grafted Nanorods in Homopolymer Films: Theory and Experiment. Macromolecules 46**,** 2856–2869 (2013).
S. M. Hur, A. L. Frischknecht, D. L. Huber, and G. H. Fredrickson, Self-assembly in a mixed polymer brush with inhomogeneous grafting density composition. Soft Matter 9**,** 5341–5354 (2013).
D. S. Bolintineanu, M. J. Stevens, and A. L. Frischknecht, Atomistic simulations predict a surprising variety of morphologies in precise ionomers, ACS Macro Lett. 2, 206 (2013).
A. D. Price, S. M. Hur, G. H. Fredrickson, A. L. Frischknecht, and D. L. Huber, Exploring lateral microphase separation in mixed polymer brushes by experiment and self-consistent field theory simulations, Macromolecules 45, 510 (2012).
M. J. A. Hore, A. L. Frischknecht, and R. J. Composto, Nanorod assemblies in polymer films and their dispersion-dependent optical properties, ACS Macro Lett. 1, 115 (2012).
L. M. Hall, M. E. Seitz, K. I. Winey, K. L. Opper, K. B. Wagener, M. J. Stevens, and A. L. Frischknecht, Ionic aggregate structure in ionomer melts: effect of molecular architecture on aggregates and the ionomer peak, J. Am. Chem. Soc. 134, 574 (2012).

Synergistic Activities
Honors
Employee Recognition Award for Individual Technical Excellence, Sandia National Laboratories (2013)
Fellow of the American Physical Society (2012)
UC President's Dissertation Year Fellowship (1997-1998)
UCSB Doctoral Scholar Fellowship (1996-1997)
NSF Fellowship (1992-1995)
Publications: 57 journal articles, 1 book chapter
Professional Service

Member, AIChE Institute Awards Committee, 2015-2019
Member-at-Large, Executive Committee of the Division of Polymer Physics, American Physical Society, 2013-2015
Editorial Advisory Board, Macromolecules and ACS Macro Letters, 2012-2014
Reviewer for: DOE-BES, NSF, Phys. Rev. Lett., Macromolecules, ACS Macro Lett., J. Chem. Phys., Soft Matter

Selected Recent Invited Talks
"Ionic Aggregation and Dynamics in Ionomer Melts: Insights from Molecular Simulations," Telluride Science Research Conference on Polymer Physics, Telluride, Colorado, June 24, 2015.
"Polymer Brush-Mediated Interactions in Nanorod-Polymer Composites," High Polymer Research Group 55th Meeting, Pott Shrigley, United Kingdom, April 28, 2015.
"Simulations of Ion Aggregation and Transport in Ion-Containing Polymers," Gordon Research Conference on Macromolecular Materials, Ventura, California, January 11, 2015.
"Simulations of Ionic Aggregation in Ionomer Melts," AIChE Annual Meeting, Atlanta, Georgia, November 20, 2014.
"Atomistic Simulations of Aggregation in Ionomer Melts," APS March Meeting, Denver, Colorado, March 5, 2014.

Collaborators: (last 4 years, outside of Sandia): P. J. Atzberger (UC Santa Barbara), R. J. Composto (U Penn), G. H. Fredrickson (UC Santa Barbara), M.J.A. Hore (Case Western), M. E. Mackay (Univ of Delaware), J. D. McCoy (NM Tech), G. Raos (Milano), J. Runt (Penn State), C. J. Soles (NIST), K. B. Wagener (Univ of Florida), K. I. Winey (U Penn)

Graduate and Postdoctoral Advisors:
James S. Langer and Glenn H. Fredrickson, UC Santa Barbara (Ph.D. advisors); Scott T. Milner, Penn State (postdoc advisor); John G. Curro, University of New Mexico (postdoc advisor).

Thesis Advisor and Postgraduate-Scholar Sponsor: (over the last 5 years)
Students: none
Postdocs: Venkat Padmanabhan (Indian Institute of Technology, Kharagpur), Lisa M. Hall (Ohio State University), Christopher A. Lueth (Fluent), Dan S. Bolintinenau (Sandia National Laboratories), Christina L. Ting, Truman Fellow (Sandia National Laboratories), K. Michael Salerno (Sandia National Laboratories), L. J. Abbott (Sandia National Laboratories)
Total: 7 postdocs, 0 students

NORMAND A. MODINE
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Email : namodin@sandia.gov

Education
Ph.D. Physics, Harvard University, November 1996
A.M. Physics, Harvard University, June 1992
B.S. Physics and B.S. Mathematics, Virginia Polytechnic Institute and State University, June 1990

Professional Experience:
Thrust Leader for CINT TSNP thrust, Sandia National Laboratories, January 2009-2013
Principal Member of the Technical Staff, Sandia National Laboratories, October 2003 - Present
Senior Member of the Technical Staff, Sandia National Laboratories, July 2000 -October 2003
Postdoctoral Researcher, Sandia National Laboratories, May 1998 - July 2000
Postdoctoral Researcher, Harvard University, November 1996 - April 1998
Postdoctoral Researcher, Rutgers University, October 1996 - November 1996
Research Staff, Harvard University, July 1996 - October 1996
Research Assistant, Harvard University, Fall 1993 - June 1996
Teaching Fellow, Harvard University, Fall 1994
Undergraduate Research Fellow, Oak Ridge National Laboratory, Summer 1989

Publications
Representing the Thermal State in Time-Dependent Density Functional Theory, N. A. Modine and R. M. Hatcher, Journal of Chemical Physics 142, 204111 (2015).
Bonding Between Graphene and MoS2 Monolayers without and with Li Intercalation, T. Ahmed, N. A. Modine, and J.-X. Zhu, Applied Physics Letters 107, 043903 (2015).
Bounds on the Range of Density-Functional-Theory Point-Defect Levels in Semiconductors and Insulators, N. A. Modine and A. F. Wright, Computational Materials Science 92, 431 (2014).
Application of the Bounds-Analysis Approach to Arsenic and Gallium Antisite Defects in Gallium Arsenide, A. F. Wright and N. A. Modine, Physical Review B 91, 014110 (2015).
First-Principles Survey of the Structure, Formation Energies, and Transition Levels of As-interstitial Defects in InGaAs, S. R. Lee, A. F. Wright, N. A. Modine, C. C. Battaile, S. M. Foiles, J. C. Thomas, and A. Van der Ven, Physical Review B 92, 045205 (2015).
Phase Stability Analysis of the InAs/GaAs (001) Wetting Layer from First Principles, J. C. Thomas, J. M. Millunchick, A. Van der Ven, and N. A. Modine, Physical Review B 89, 205306 (2014).
Considerations for Surface Reconstruction Stability Prediction on GaAs (001), J. C. Thomas, A. Van der Ven, J. M. Millunchick, and N. A. Modine, Physical Review B 87, 075320 (2013).
Systematic Approach for Determination of Equilibrium Atomic Surface Structure, J. C. Thomas, N. A. Modine, J. M. Millunchick, and A. Van der Ven, Physical Review B 82, 165434 (2010).
Determining the GaSb/GaAs-(2x8) Reconstruction, J.E. Bickel, N.A. Modine, and J. M. Millunchick, Surface Science 603, 2945 (2009).
Surface Atomic Order of Compound III-V Semiconductor Alloys at Finite Temperature, J.C. Thomas, J. M. Millunchick, N.A. Modine, and A. Van der Ven, Physical Review B 80, 125315 (2009).

Synergistic Activities
Publicly Available Software:
ACRES: Adaptive Coordinate Real-space Electronic Structure, N. A. Modine, G. Zumbach, U. V. Waghmare, G. S. Smith, M. Chen, H. Kim, and E. Kaxiras, Distributed by the Department of Defense Common High-Performance Software Support Initiative.
HARES: High-performance-fortran Adaptive-grid Real-space Electronic Structure, U. V. Waghmare, Hanchul Kim, I. J. Park, N. A. Modine, P. Maragakis, G. Zumbach, and E. Kaxiras, Distributed by the

National Nanotechnology Infrastructure Network.
Socorro Electronic-Structure Software, A. F. Wright, N. A. Modine, R. A. Lippert, Ryan Hatcher, Alan Tackett, A. E. Mattsson, S. M. Foiles, M. P. Sears, R. P. Muller, and S. J. Plimpton, Copyright (2002) Sandia Corporation.

Collaborators (last 48 months): Sandia National Laboratories: A. F. Wright, S. R. Lee, C. C. Battaile, S. M. Foiles, S. M. Myers, W. R. Wampler, C. Chan, A. M. Armstrong, M. H. Crawford, W. W. Chow; Los Alamos National Laboratory: J.-X. Zhu, T. Ahmed; Harvard University: E. Kaxiras, M. Stopa; University of Michigan, Ann Arbor: J. M. Millunchick, C. R. Tait, E. Anderson, A. Duzik; University of California, Santa Barbara: A. Van der Ven, J. C. Thomas; University of New Mexico: S. Krishna, T. Garwood; Samsung Corporation: R. M. Hatcher

Graduate and Postdoctoral Advisors:
Graduate and Postdoctoral Advisor: E. Kaxiras, Harvard University
Postdoctoral Advisor: D. Vanderbilt, Rutgers University

Thesis Advisor and Postgraduate-Scholar Sponsor: (over the last 5 years)
Students: C. R. Tait, Michigan; T. Garwood, New Mexico (undergraduate); J. C. Thomas, Michigan; A. Duzik, Michigan
Total: 0 postdocs, 4 students

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Education

Undergraduate:	University of Cincinnati	Physics, B.S., Math, B.A. 1984
Graduate:	The Johns Hopkins University	Physics, 1991

Professional Experience:
Thrust Leader, CINT, Sandia National Laboratories, 2006-2008
Member of Technical Staff, Sandia National Laboratories, Feb 1997 – present
Limited Term Appointee, Sandia National Laboratories, July 1995 – Feb 1997
Postdoctoral Fellow, Exxon Research and Engineering Co., Jan 1993 – July 1995
Postdoctoral Fellow, Forschungszentrum Juelich, Oct 1991 – Dec 1992

Publications

S. G. Moore, Mark J. Stevens and G.S. Grest, "Liquid-vapor interface of the Stockmayer fluid in a uniform external field," Phys. Rev. E 91, 022309 (2015).
C. Buitrago, D. Bolintineanu, M. Seitz, K. Opper, K. Wagener, Mark Stevens, A. Frischknecht and K. Winey, "Direct Comparisons of X-ray Scattering and Atomistic Molecular Dynamics Simulations for Precise Acid Copolymers and Ionomers," Macromolecules 48, 1210 (2015).
C. L. Ting, Mark J. Stevens and A. L. Frischknecht, "Structure and dynamics of coarse-grained ionomer melts under an external electric field," Macromolecules 48, 809 (2015).
Z. Cao, Mark Stevens, J.-M. Carrillo and A. Dobrynin, "Adhesion and Wetting of Soft Nanoparticles on Textured Surfaces: Transition between Wenzel and Cassie-Baxter States," Langmuir 31, 1693 (2015).
Z. Cao, Mark J. Stevens and A. V. Dobrynin, "Elastocapillarity: Adhesion and Wetting in Soft Polymeric Systems," Macromolecules 47, 6515 (2014).
Z. Cao, Mark J. Stevens and A. V. Dobrynin, "Adhesion and Wetting of Nanoparticles on Soft Surfaces, Macromolecules 47, 3203 (2014).
D.S. Bolintineanu, Mark J. Stevens and A.L. Frischknecht, "Atomistic Simulations Predict a Surprising Variety of Morphologies in Precise Ionomers," ACS Macro Letters 2, 206 (2013).
Mark J. Stevens, D. B. McIntosh and O. A. Saleh, "Simulations of Stretching a Strong, Flexible Polyelectrolyte: Using long chains to access the Pincus Scaling Regime," Macromolecules 46, 6369 (2013).
Mark J. Stevens, D. B. McIntosh and O. A. Saleh, "Simulations of Stretching a Strong, Flexible Polyelectrolyte," Macromolecules 45, 5757, (2012).
L. Hall, M. Seitz, K. Winey, K. Opper, K. Wagener, Mark J. Stevens, A. Frischknecht, "Ionic Aggregate Structure in Ionomer Melts: Effect of Molecular Architecture on Aggregates and the Ionomer Peak," J. Am. Chem. Soc. 134, 574 (2012).

Synergistic Activities
APS DCOMP Member-at-Large 03/15 - 02/18
Fellow of the American Physical Society, 2010
Sandia Outstanding Mentor Award, 2012

Collaborators: Andrej Dobrynin (U. Akron), Omar Saleh (UCSB), Jeffrey Sokoloff (Northeastern), Ken Wagener (U. Florida), Karen Winey (U. Penn)
Graduate and Postdoctoral Advisors: Mark Robbins, Johns Hopkins University (Ph.D. Advisor), Kurt Kremer, Max Planck Institute, Mainz, Germany and Gary S. Grest, Exxon Research and Engineering (now at Sandia) (Postdoctoral Advisors).

Thesis Advisor and Postgraduate Scholar - Sponsor:
Postdocs at Sandia: Dan Bolintineanu, Shengfeng Cheng, Lisa Hall, Allison Dickey, Dina Mirijanian, Ashley Tucker,
Students: Ankush Aggrawal (UCLA), Edward Trigg (U. Penn)
Total: 6 postdocs, 2 students

SERGEI TRETIAK
Staff Scientist
Center for Integrated Nanotechnolgies
Los Alamos National Laboratories
Los Alamos, NM 87545

Phone: 505-667-8351
Fax: 505-665-3909
Email: serg@lanl.gov

Education

1999 Ph.D. in Chemistry, University of Rochester (Rochester, NY); Advisor: Prof. Shaul Mukamel
1994 M.S. in Physics (Highest Honors), Institute of Physics and Technology (Moscow, Russia)

Professional Experience:

2001 – Present	Technical Staff Member, Theoretical Division, LANL
2005 – Present	Staff Scientist, Center for Integrated Nanotechnologies (CINT), LANL/SNL
2015 – Present	Adjunct Professor at the University of California, Santa Barbara, CA
2015 – Present	Adjunct Professor at Skolkovo Institute of Science & Technology (Russia)
2013 – 2015	Founding Faculty Fellow at Skolkovo Institute of Science & Technology (Russia)
2006 – 2007	CNRS invited professor position, UMR 6510, University of Rennes, France
1999 – 2001	Director's Postdoctoral Fellow, Theoretical Division, LANL
1999 – 1999	Postdoctoral Associate, University of Rochester (Rochester, NY)
1994 – 1999	Graduate Student, University of Rochester (Rochester, NY)
1991 – 1994	Graduate Student, Institute of Spectroscopy of Russian Academy of Sciences

Publications (out of ~200, citation index ~9000, H-index ~50):

S. Kilina, D. Kilin, S. Tretiak, Light-Driven and Phonon-Assisted Dynamics in Organic and Semiconductor Nano-Structures, Chemical Reviews, 115, 5929 (2015).

W. Nie, T. Hsinhan, R. Asadpour, J.C. Blancon, R. Kappera, M. Chhowalla, A. Neukirch, S. Tretiak, G. Gupta, J. Crochet, M.A. Alam, H.-L. Wang and A.D. Mohite, High-efficiency solution-processed perovskite solar cells with millimeter-scale grains, Science, 347, 522 (2015).

L. Adamska, I. Nayyar, N. Oldani, S. Fernandez-Alberti, H. Chen, A.K. Swan, S.K. Doorn, S. Tretiak, Self-trapping of excitons, violation of Condon approximation and efficient fluorescence in conjugated cycloparaphenylenes, Nano Letters, 14, 6539 (2014).

T. Nelson, S. F. Alberti, A. Roitberg, and S. Tretiak, Nonadiabatic Excited-State Molecular Dynamics: Modeling photophysics in organic conjugated materials Accounts Chemical Research, 47, 1155 (2014).

V. N. Gorshkov, S. Tretiak, and D. Mozyrsky, Semiclassical Monte-Carlo approach for modeling non-adiabatic dynamics in extended molecules, Nature Communications, 4, 2114 (2013).

J. Clark, T. Nelson, S. Tretiak, G. Cirmi, and G. Lanzani, Femtosecond Torsional Relaxation, Nature Physics, 8, 225-231 (2012).

F. Terenziani, C. Katan, M. Blanchard-Desce, E. Badaeva, and S. Tretiak, Enhanced two-photon absorption of organic chromophores: theoretical and experimental assessments, Adv. Mat. (Review Article, journal cover page) 20, 1-38 (2008).

C. Wu, S. Malinin, S. Tretiak, V. Chernyak, Multiscale modeling of electronic excitations in branched conjugated molecules using exciton scattering approach, Phys. Rev. Lett. 100, 057405 (2008).

C. Wu, S. Malinin, S. Tretiak, and V. Chernyak, Exciton scattering and localization in branched dendrimeric structures, Nature Physics 2, 631-635 (2006).

S. A. Crooker, J. Hollingsworth, S. Tretiak, and V. I. Klimov, Spectrally resolved dynamics of energy transfer in quantum-dot assemblies: Towards engineered energy flows in artificial materials, Phys. Rev. Lett., 89, 6802-6802 (2002).

Synergistic Activities

Organizer of the conferences in the Center for Nonlinear Studies (CNLS) at LANL: "Excited State Processes in Electronic and Bio Nanomaterials (ESP)", 2001, 2003, 2005, 2007, 2009, 2011, 2014, 2016;

Co-Organizer of the CNLS Conferences:"Statistical Physics of Macromolecules: from electronic structure to

fluid mechanics", Santa Fe, NM, 2004;"Electronic and Vibrational Interactions in Carbon Nanotubes", Santa Fe, NM, 2007; "Energy for 21st century", Santa Fe, NM, 2009.

Co-organizer of the session "Physical Chemistry of Interfaces and Nanomaterials" for the SPIE Nano Science and Engineering conference, San Diego, CA, 2007-2016.

Co-Organizer of Telluride workshop on "Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy", Telluride, CO, 2007, 2009, 2011, 2013, 2015.

Member of LANL Postdoctoral Committee (2006-2009), Los Alamos National Laboratory, 2006-2009; Member of LDRD-ER review committee in Quantum & Optical Science (2011-2013), Chemistry and Materials category (2005), in Technology category (2004), Los Alamos National Laboratory;

Reviewer for about 20 major peer-reviewed journals and several funding agencies (NSF, Petroleum Research Fund (ACS), DOE BES, US Department of State for the Science Centers, etc.).

Honors

LANL Postdoctoral Distinguished Mentor (2015), APS Fellow (2014), LANL Fellows Prize (2010), Slansky Fellow Award (2001), LANL Director's Postdoctoral Fellow (1999-2001), Arnold Weissberger Fellow (1997-1998), Graduate Student Award in Computational Chemistry (1996), Elon Huntington Hooker Fellow (1996-1997), Sherman Clarke Fellow (1996-1997), Diploma with Honor, Moscow Institute of Physics and Technology (1994).

Selected recent invited and keynote talks (out of about 130):

249th ACS National Meeting, Denver (2015); MRS Fall Meeting, Boston (2014); APS March Meeting, Denver (2014); MRS Fall Meeting, Boston (2013); Optical probes (OP-2013), Durham, UK (2013); 22nd I-APS meeting, Sarasota, FL (2013), 243th ACS National Meeting, San Diego, CA (2012), 52th Sanibel Symposium, St. Simons (2012), 242th ACS National Meeting, Denver, CO (2011), PacifiChem, Honolulu HI (2010); CCTCC-19, Jackson, MS, (2010); CECAM, Ireland, (2010); 237th ACS National Meeting, Salt Lake City (2009); Telluride Workshop, CO (2007, 2009, 2011); 92nd OSA National Meeting, Rochester (2008); 235th ACS National Meeting, New Orleans (2008); APS March Meeting, New Orleans (2008).

Collaborators: within LANL: D. L. Smith, R. L. Martin, A. Saxena, A.R. Bishop, A. Mohite, S.K. Doorn, H. Htoon, D. Dattelbaum, H.L. Wang, S.D. McGrain, A.V. Balatsky, A. Piryatinski, D. Mozyrsky, V. Klimov.
outside LANL: S. Mukamel (UC Irvine), G.C. Bazan (UC Santa Barbara), A. Myers-Kelley (UC Merced), J. Perry, (GaTech), J. Lupton (Germany), V. Chernyak (Wayne State U.), M. Blanchard-Desce (France), F. Furche (UCI), O. Prezhdo (U. Rochester), G. Lanzani (Italy), G.D. Scholes (Princeton), A. Jorio (Brazil), S. Fernandez-Alberti (Argentina), A. Roitberg (U. Florida), A. Shreve (UNM), Y. Zhao (Singapore).

Graduate and Postdoctoral Advisors: Shaul Mukamel, University of California, Irvine (Ph.D. Advisor). Alan Bishop, LAN (Postdoctoral Advisor)

Thesis Advisor and Postgraduate – Scholar Sponsor: (T-1/CNLS) Postdoc Advisees: A. Masunov, 2001-2004, currently faculty at USF, R. Magyar, 2003-2005, currently TSM at SNL; A. Piryatinski, 2002-2006, currently TSM at LANL; S. Goupalov, 2003-2004, currently faculty at JSU; M. Lucero, 2005-2006, M. Galperin, 2007-2008, currently faculty at UC San Diego; J. Tao, 2007-2010, currently faculty at Tulane U; S. Kilina, 2008-2010, currently faculty at NDSU, K. Velizhanin, 2010-2012, currently TSM at LANL; H. Li (2011-2014, currently postdoc at U Houston), A. Zhugayevych (2011-2014, currently faculty at Skoltech, Moscow); A. Roslyak (2012-2014, currently faculty at Fordham U), T. Nelson (Feynman Fellow, 2013-present), L. Adamska (2013-present), J. Bjorgaard (2013-present). A. White (2014-present), A. Neukirch (2014-present). (Under)Graduate Advisees: J. Vogel (NDSU), M. Belyanchikov (MSU), A. Sifain (USC), D. Svetlov (USC), J. Liu (USC), O. Masaleva (MSU). N. Dandu (NDSU), R. Neeman (TTU), S. Matveev (MSU), C. Chuang (MIT), A. Naumov (Skoltech), K. Kalinin (Skoltech), K. Liu (Wayne State), Eli Chertkov (Princeton), O. Postupna (U Rochester), T. Van der Poll (UCSB), J. Coughlin (UCSB), T. Nelson (U. Rochester), I. Nayyar (UCF), J. McClean (Harvard), R. Paradez (U. Houston), C. Legaspi (Carnegie-Melon), G. Kolesov (U. Wyoming), T. Shi (Wayne State), C. Olson (NDSU), O. Postupna (U. Rochester), T. Kuznetsova (Harvard), J. Klesko (Wayne State), A. White (UCD), S. Fischer (UW), A. Crotty (UCF), S.

Goel (UCF), A. Furmanchuk (Jackson State), J. Ramirez (UF), C. Thacker (UF), Hao Li (Wayne State), E. Badaeva (UW), Th. Koerzdoerfer (Max Plank, Germany), V. Albert (UF), S. Difley (MIT), K. Velizhanin (LANL), C. Wu (Notre Dame), S. Kilina (LANL), C. Isborn (CalTech), P. Yang (PNNL), S. Ponomarev (Wesleyan), S. Kurennoy (UC Santa Barbara), C. Craig (Western Washington), E. Heatwole (Humboldt), K. Igumenshchev (U. Rochester), I. Franco (Northwestern), N. Kobko (CUNY), A. Moran (UNC), T. Humble (U. Oregon)

Supervised 17 postdoctoral associates/fellows and mentored over 60 graduate students at LANL

STUART A. TRUGMAN
Staff Scientist
Center for Integrated Nanotechnologies
Los Alamos National Laboratory
Los Alamos, NM 87545

Phone: 505-667-0208
Fax: 505-665-4063
Email: sat@lanl.gov

Education

Undergraduate:	B.A. in Chemistry and Physics (highest honors), Harvard University, 1976
Graduate:	Ph.D. in Physics, Stanford University, 1982

Professional Experience:

Staff Member, T-11 and T-4, Los Alamos National Laboratory, August 1986 to present
Assistant Professor of Physics, Princeton University, September 1984 to July 1986
Postdoctoral Fellow, Cornell University, September 1982 to August 1984
IBM Postdoctoral Fellow, Stanford University, January 1982 to August 1982
NSF Fellow, Stanford University, September 1976 to September 1979

Publications (out of ~170, citation index ~5000, h-index 37):

Using ultrashort optical pulses to couple ferroelectric and ferromagnetic order in an oxide heterostructure, Y. M. Sheu,
S. A. Trugman, L. Yan, Q. X. Jia, A. J. Taylor, and R. P. Prasankumar, Nature Comm. 5, 5832 (2014).

The influence of charge and magnetic order on polaron and acoustic phonon dynamics in $LuFe_2O_4$, J. Lee, S. A.
Trugman, C. L. Zhang, D. Talbayev, X. S. Xu, S.-W. Cheong, D. A. Yarotski, A. J. Taylor and R. P. Prasankumar,
Appl. Phys. Lett. 107, 042906 (2015).

Ultrafast carrier dynamics in the large magnetoresistance Material WTe_2, Y. M. Dai, J. Bowlan, H. Li, H. Miao, S. F.
Wu, W. D. Kong, Y. G. Shi, S. A. Trugman, J.-X. Zhu, H. Ding, A. J. Taylor, D. A. Yarotski, and R. P. Prasankumar, Phys. Rev. B 161104(R) (2015).

Polaronic transport induced by competing interfacial magnetic order in a $La_{0.7}Ca_{0.3}MnO_3$ / $BiFeO_3$ heterostructure, Y.
M. Sheu, S. A. Trugman, L. Yan, J. Qi, Q. X. Jia, A. J. Taylor, and R. P. Prasankumar, Phys. Rev. X 4, 021001
(2014).

Relaxation dynamics of the Holstein polaron, D. Golez, J. Bonca, L. Vidmar, and S. A. Trugman, Phys. Rev. Lett. 109, 236402 (2012).

Optical tuning and ultrafast dynamics of high-temperature superconducting terahertz metamaterials, R. Singh, A. K. Azad, H.-T. Chen, Q. X. Jia, A. J. Taylor, S. A. Trugman, J. Xiong, and H. Yang, Nanophotonics 1, 117 (2012).

Coexistence of coupled magnetic phases in epitaxial TbMnO3 films revealed by ultrafast optical spectroscopy, J. Qi, L. Yan, H. D. Zou, J.-X. Zhu, S. A. Trugman, A. J. Taylor, Q. X. Jia, and R. P. Prasankumar, Appl. Phys. Lett. 101, 122904 (2012).

Ultrafast hopping dynamics of 5f electrons in the Mott insulator UO2 studied by femtosecond pump-probe spectroscopy, Y. Q. An, A. J. Taylor, S. D. Conradson, S. A. Trugman, T. Durakiewicz, and G. Rodriguez, Phys. Rev. Lett. 106, 207402 (2011).

Quantum dynamics of polaron formation, Li-Chung Ku and S. A. Trugman, Phys. Rev. B 75, 014307 (2007).

The Effect of Inelastic Processes on Tunneling, J. Bonca and S. A. Trugman, Phys. Rev. Lett. 75, 2566 (1995).

Synergistic Activities

Research Experience: Theoretical condensed matter physics, including nanotechnology, strongly correlated systems, quantum dynamics, time-resolved spectroscopy, polarons, colossal magnetoresistance, high

temperature superconductivity, inelastic tunneling, heavy fermions, the quantum Hall effect, and linear and nonlinear transport in novel and disordered materials.

Reviewer for about 10 major peer-reviewed journals and several funding agencies (NSF, DOE BES, etc.)
Co-organizer for Nanowires symposium, CINT user conference, Albuquerque, NM, 2012.
Site Reviewer, LBNL, 2013.

Honors:
Los Alamos Fellows Prize for outstanding research, 1996.
Yu-Miin Sheu, postdoc co-advisee, awarded the LANL Postdoctoral Publication Prize in Experimental Sciences, 2015.

Collaborators (last 48 months):

R. D. Averitt (UCSD), J. Bonca (J. Stefan Inst., Slovenia), S.-W. Cheong (Rutgers), S. D. Conradson (Soleil, France), G. L. Dakovski (SLAC), D. Golez (U. Fribourg, Switzerland), N. Grady (Sandia, NM), J. Lee (S. Korea), M. Mierzejewski (U. Silesia, Poland), J. Mustre de Leon (Cinvestav, Mexico), John O'Hara (Oklahoma State), J. Qi (Sichuan U., PRC), Yu-Miin Sheu (National Chiao Tung U., Taiwan), D. Talbayev (Tulane), T. A. Tyson (NJIT, NJ), R. Valdes-Aguilar (Ohio State), L. Vidmar (Penn. State)

Graduate and Postdoctoral Advisors: PhD advisor, Sebastian Doniach, Stanford University; Postdoc advisor, John Wilkins, Ohio State Univ.

Thesis Advisor and Postgraduate-Scholar Sponsor: (over the last 5 years)
Postdocs mentored or co-mentored at LANL: Pam Bowlan, John Bowlan, Yaomin Dai, Jinho Lee, Yu-Miin
Sheu, Jingbo Qi, Michael Galperin, Yong An
Total number of postdocs mentored or co-mentored in the last 5 years: 8

9.0 Other Support of Investigators and Collaborators

Investigator: Jian-Xin Zhu (Jia)	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Pending	
Project/Proposal Title and grant number, if appropriate: Integrated Modeling of Novel Materials	
Source of Support: BES	Location of Project: LANL
Annual Award Amount: $18M	Total Award Period Covered: 10/13-09/16
Annual Award Amount to PI's Research: $250k	
Person-Months Per Year Committed to Project: 6C Pers. Months; Specify: Cal., Acad., or Sumr: C	
Describe research including synergies and/or overlaps with This Proposal/Award: CINT is a joint Sandia-LANL BES User Facility whose charter is to explore the basic science associated with the integration of nanomaterials into complex systems and composites. Jian-Xin's role is the development and application of first-principles electronic structure approach to describe the composite materials with electronic correlations and quantum transport in nanoscale and low-dimension, and support of user projects in these areas.	
Investigator: Jian-Xin Zhu (Janoschek)	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Pending	
Project/Proposal Title and grant number, if appropriate: A new approach to mesoscale functionality: Emergent tunable superlattices	
Source of Support: LDRD-DR	Location of Project: LANL
Annual Award Amount: $1.8M	Total Award Period Covered: 10/14-09/17
Annual Award Amount to PI's Research: $25K	
Person-Months Per Year Committed to Project: 0.6C Pers. Months; Specify: Cal., Acad., or Sumr:	
Describe research including synergies and/or overlaps with This Proposal/Award: Develop electronic structure underpinning for the effective modeling of skyrmions. There is no overlap with this proposal.	
Investigator: Jian-Xin Zhu (Yarotski)	Other Agencies to which this proposal has been/will be submitted:

Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: Multiferroic Response Engineering in Mesoscale Oxide Structures	
Source of Support: LDRD-DR	Location of Project: LANL
Annual Award Amount: $1.8M	Total Award Period Covered: 10/13-09/16
Annual Award Amount to PI's Research: $75K	
Person-Months Per Year Committed to Project: 1.8C Pers. Months; Specify: Cal., Acad., or Sumr: C	
Describe research including synergies and/or overlaps with This Proposal/Award: Provide underpinning theory for multiferroic response in mesoscale oxide structures. Synergistic with current proposal.	
Investigator: Jian-Xin Zhu (Crockett)	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: ASC Physics and Modeling: Equation of State	
Source of Support: NNSA-ASC	Location of Project: LANL
Annual Award Amount: $1.5M	Total Award Period Covered: 10/15-09/16
Annual Award Amount to PI's Research: $150K	
Person-Months Per Year Committed to Project: 4 C Pers. Months; Specify: Cal., Acad., or Sumr:	
Describe research including synergies and/or overlaps with This Proposal/Award: Provide cold curves by performing electronic structure calculations.	

Investigator: Amalie Frischknecht (Hongyou Fan, PI)	Other Agencies to which this proposal has been/will be submitted: none
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: Molecular Nanocomposites	
Source of Support: DOE BES MS&E	Location of Project: Sandia National Labs
Annual Award Amount: $1400k	Total Award Period Covered:10/1/02 - present
Annual Award Amount to PI's Research: $70k	

Person-Months Per Year Committed to Project: _1.8_ Pers. Months (Calendar)	
Describe research including synergies and/or overlaps with This Proposal/Award: To explore the use of energy consuming, switchable, and/or responsive components to create programmable and/or reconfigurable nanocomposites. This work is complementary to my work in CINT but focuses on different systems.	
Investigator: Amalie Frischknecht (PI: George Karniadakis, Brown University)	Other Agencies to which this proposal has been/will be submitted: none
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: Collaboratory on Mathematics for Mesoscopic Modeling of Materials (CM4)	
Source of Support: DOE NNSA	Location of Project: Sandia National Labs
Annual Award Amount: $3M ($750K to SNL)	Total Award Period Covered: 10/12-9/17
Annual Award Amount to PI's Research: $108k	
Person-Months Per Year Committed to Project: 3.0 Pers. Months (Calendar)	
Describe research including synergies and/or overlaps with This Proposal/Award: The Collaboratory on Mathematics for Mesoscopic Modeling of Materials (CM4) focuses on developing rigorous mathematical foundations for understanding and controlling fundamental mechanisms in mesoscale processes to enable scalable synthesis of complex materials, through the design of efficient modeling methods and corresponding scalable algorithms. My work on this project is focused on multiscale modeling of electrokinetic phenomena and does not overlap with this FWP.	

Investigator: Amalie Frischknecht (PI: Amalie Frischknecht)	Other Agencies to which this proposal has been/will be submitted: none
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: Understanding Transport and Aging Mechanisms to Optimize Sandia's Ion-conducting Electrolytes for Energy Applications	
Source of Support: Sandia National Laboratories, Laboratory Directed Research and Development (LDRD) Program	Location of Project: Sandia National Labs
Annual Award Amount: $460K	Total Award Period Covered: 10/12-9/15
Annual Award Amount to PI's Research: $80k	
Person-Months Per Year Committed to Project: 1.2 Pers. Months (Calendar)	
This project is focused on understanding molecular phenomena in a class of proton-conducting block copolymers. For this project I am conducting molecular dynamics simulations of the polymer, water and ion	

transport in the polymer, and of the effects of chemical changes on mechanical properties. This work does not overlap with this FWP.

Investigator: Normand Modine (L. Lorence, PI)	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: Qualification Alternatives to the Sandia Pulsed Reactor	
Source of Support: NNSA ASC P&EM Location of Project: Sandia National Laboratories, Albuquerque, NM	
Total Award Amount: $2,000K/year	Total Award Period Covered: FY15-16
Total Award Amount to PI's Research: $200K	
Describe Synergies and/or Overlaps with This Proposal/Award: This work involves theoretical studies of carrier-capture processes at defects in semiconductors. This work aligns with my work on carrier-defect interactions in CINT, and some of my co-Investigators on this project are CINT Users.	
Person-Months Per Year Committed to Project: _2_ Pers. Months; Specify: Cal.	
Investigator: Normand Modine (A. Wright, PI) Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: Compact Models for Defect Diffusivity in Semiconductor Alloys	
Source of Support: Sandia LDRD Location of Project: Sandia National Laboratories, Albuquerque, NM	
Total Award Amount: $1,400K	Total Award Period Covered: FY15-17
Total Award Amount to PI's Research: $330K	
Describe Synergies and/or Overlaps with This Proposal/Award: The proposed work would develop fundamental techniques to calculate defect properties in semiconductor alloys. The DFT/cluster expansion/Monte-Carlo approach used in this project was developed as part of my CINT work, but in this project, this approach is applied to study defects in alloys, while in my CINT research they have been applied to determine the structure of surfaces and interfaces.	
Person-Months Per Year Committed to Project: _4_ ; Specify: Cal.	

Investigator: Mark Stevens (Hongyou Fan, PI)	Other Agencies to which this proposal has been/will be submitted: none
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	

Project/Proposal Title and grant number, if appropriate: Molecular Nanocomposites	
Source of Support: DOE BES MS&E	Location of Project: Sandia National Labs
Annual Award Amount: $1.3M	Total Award Period Covered:10/1/02 - present
Annual Award Amount to PI's Research: $140k	
Person-Months Per Year Committed to Project: _2_ Pers. Months (Calendar)	
Describe research including synergies and/or overlaps with This Proposal/Award: To explore the use of energy consuming, switchable, and/or responsive components to create programmable and/or reconfigurable nanocomposites.	
Investigator: Mark Stevens **(George Bachand, PI)**	Other Agencies to which this proposal has been/will be submitted: None
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: Active Assembly of Dynamic and Adaptable Materials	
Source of Support: DOE BES MS&E	Location of Project:Sandia National Labs
Annual Award Amount: $1.47M	Total Award Period Covered: Oct. 1, 2000 – present
Annual Award Amount to PI's Research: $140k	
Person-Months Per Year Committed to Project: _2_ Pers. Months (Calendar)	
Describe research including synergies and/or overlaps with This Proposal/Award: To exploit key strategies used by living systems to develop materials whose transport, reconfiguration, and disassembly can be programmed or "self-directed" in controlled environments.	

Investigator: Mark Stevens, (Erica Redline PI)	Other Agencies to which this proposal has been/will be submitted: none
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: Improving Mechanical Performance of Thermosets	
Source of Support: Sandia National Laboratories, Laboratory Directed Research and Development (LDRD) Program	Location of Project: Sandia National Labs
Annual Award Amount: $ 250K	Total Award Period Covered: 10/14-9/16
Annual Award Amount to PI's Research: $40k	
Person-Months Per Year Committed to Project: 1 Pers. Months (Calendar)	

Describe research including synergies and/or overlaps with This Proposal/Award: To investigate new strategies for synthesizing thermoset polymers.

Investigator: Sergei Tretiak (Mohite)	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: "Perovskite solar cells: the next frontier in energy harvesting"	
Source of Support: LANL LDRD ER	Location of Project: LANL
Total Award Amount: $ $1M	Total Award Period Covered: 10/2014-10/2017
Total Award Amount to PI's Research: $1M	
Describe Synergies and/or overlaps with This Proposal/Award: The above project aims to develop novel hybrid perovskite materials for efficient and photostable solar cells. Theoretical methods used in the research to calculate band structure and optical properties of perovskites.	
Person-Months Per Year Committed to Project: _1___ Pers. Months; Specify: Cal., Acad., or Sumr: Cal.	
Investigator: Sergei Tretiak (Scharff)	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: "Photoactive Energetic Materials for Quantum Optical Initiation"	
Source of Support: LANL LDRD DR	Location of Project: LANL
Total Award Amount: $5.2M	Total Award Period Covered: 10/2013-10/2016
Total Award Amount to PI's Research: $5.2M	
Describe Synergies and/or overlaps with This Proposal/Award: This project focuses experimental and theoretical efforts to design novel optically sensitive energetic materials. Theoretical modeling of excited state dynamics and photochemistry aims to understand structure/property relationships of newly synthesized explosives and improve their optical properties. We anticipate that developed theoretical tools will be applicable to a broad range of nanomaterials in the focus of CINT.	
Person-Months Per Year Committed to Project: __5__ Pers. Months; Specify: Cal., Acad., or Sumr: Cal.	

10.0 Budget and Budget Explanation

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Sandia National Laboratories				**Budget Page No:**	1
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Gary Grest (TSNP Thrust Leader)				Requested Duration:	12 (FY2016) (Months)
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applpicant	by DOE
1. Grest, Gary (.75 FTE)	9.00			152,141.00	
2. Modine, Normand (.5 FTE)	6.00			83,032.00	
3. Frischknect, Amalie (.5 FTE)	6.00			79,073.00	
4. Stevens, Mark (.5 FTE)	6.00			86,985.00	
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	27.00			401,231.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	12.00			91,083.00	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				492,314.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				179,694.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				672,008.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL				0.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				672,008.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				619,820.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				1,291,828.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				1,291,828.00	0.00

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure Statement on Reverse

ORGANIZATION: Sandia National Laboratories

Budget Page No: 2

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR: Gary Grest (TSNP Thrust Leader)

Requested Duration: 12 (FY17) (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. Grest, Gary (.75 FTE)	9.00			156,090.00	
2. Modine, Normand (.5 FTE)	6.00			81,126.00	
3. Frischknect, Amalie (.5 FTE)	6.00			85,183.00	
4. Stevens, Mark (.5 FTE)	6.00			89,240.00	
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	27.00			411,639.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	12.00			93,448.00	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				505,087.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				184,357.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				689,444.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL				0.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				689,444.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				642,778.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				1,332,222.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				1,332,222.00	0.00

DOE F 4620.1
(04-93)
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U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure Statement on Reverse

ORGANIZATION: Sandia National Laboratories

Budget Page No: 3

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR: Gary Grest (TSNP Thrust Leader)

Requested Duration: 12 (FY18) (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. Grest, Gary (.75 FTE)	9.00			161,279.00	
2. Modine, Normand (.5 FTE)	6.00			83,822.00	
3. Frischknect, Amalie (.5 FTE)	6.00			88,014.00	
4. Stevens, Mark (.5 FTE)	6.00			92,205.00	
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	27.00			425,320.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	12.00			96,553.00	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				521,873.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				190,483.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				712,356.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL				0.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				712,356.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				668,013.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				1,380,369.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				1,380,369.00	0.00

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U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure Statement on Reverse

ORGANIZATION: Sandia National Laboratories

Budget Page No: 4

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR: Gary Grest (TSNP Thrust Leader)

Requested Duration: 36 (FY16-18) (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. Grest, Gary (.75 FTE)	27.00			469,510.00	
2. Modine, Normand (.5 FTE)	18.00			244,020.00	
3. Frischknect, Amalie (.5 FTE)	18.00			256,229.00	
4. Stevens, Mark (.5 FTE)	18.00			268,430.00	
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	81.00			1,238,189.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	36.00			281,084.00	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				1,519,273.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				554,535.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				2,073,808.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL				0.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				2,073,808.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				1,930,611.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				4,004,419.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				4,004,419.00	0.00

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U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION
Los Alamos National Laboratory

Budget Page No: 1

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR
Gary Grest (TSNP Thrust Leader)

Requested Duration: 12 (FY16) (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. Zhu, Jiankin (0.60FTE)	7.20			$99,342	
2. Tretiak, Sergei (0.50FTE)	6.00			$90,620	
3. Trugman, Stuart (0.50FTE)	6.00			$90,620	
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (3) TOTAL SENIOR PERSONNEL (1-6)	19.20			$280,581	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	12.00			$76,911	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$357,493	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$150,161	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$507,654	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$225,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS- University contract					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$225,000	
H. TOTAL DIRECT COSTS (A THROUGH G)				$732,654	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$628,369	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$1,361,023	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$1,361,023	

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(04-93)
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U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION
Los Alamos National Laboratory

Budget Page No: 2

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR
Gary Grest (TSNP Thrust Leader)

Requested Duration: 12 (FY17) (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. Zhu, Jianxin (0.60FTE)	7.20			$102,322	
2. Tretiak, Sergei (0.50FTE)	6.00			$93,339	
3. Trugman, Stuart (0.50FTE)	6.00			$93,339	
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (3) TOTAL SENIOR PERSONNEL (1-6)	19.20			$288,999	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	12.00			$79,219	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$368,218	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$154,666	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$522,884	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$250,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS- University Contract					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$250,000	
H. TOTAL DIRECT COSTS (A THROUGH G)				$772,884	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$651,699	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$1,424,583	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$1,424,583	

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(04-93)
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U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure Statement on Reverse

ORGANIZATION
Los Alamos National Laboratory

Budget Page No: 3

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR
Gary Grest (TSNP Thrust Leader)

Requested Duration: 12 (FY18) (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Zhu, Jianxin (0.60FTE)	7.20			$105,391	
2. Tretiak, Sergei (0.50FTE)	6.00			$96,139	
3. Trugman, Stuart (0.50FTE)	6.00			$96,139	
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (3) TOTAL SENIOR PERSONNEL (1-6)	19.20			$297,669	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	12.00			$81,595	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$379,264	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$159,306	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$538,570	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$275,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS- University Contract					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$275,000	
H. TOTAL DIRECT COSTS (A THROUGH G)				$813,570	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$675,549	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$1,489,119	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$1,489,119	

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(04-93)
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U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION
Los Alamos National Laboratory

Budget Page No: 4

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR
Gary Grest (TSNP Thrust Leader)

Requested Duration: 36 (FY16-18) (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. Zhu, Jianxin (0.60FTE)	21.60			$307,054	
2. Tretiak, Sergei (0.50FTE)	18.00			$280,098	
3. Trugman, Stuart (0.50FTE)	18.00			$280,098	
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (3) TOTAL SENIOR PERSONNEL (1-6)	57.60			$867,249	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	36.00			$237,725	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$1,104,975	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$464,133	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$1,569,108	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$750,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$750,000	
H. TOTAL DIRECT COSTS (A THROUGH G)				$2,319,108	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$1,955,617	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$4,274,725	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$4,274,725	

10. Budget Explanation

A. Senior Personnel

Amalie Frischknecht – (CINT Scientist) Provides support for approved CINT user projects and conducts independent research in support of CINT internal science program.

Gary Grest – (TSNP Thrust Leader) Provides scientific leadership for Thrust, provides support for approved CINT user projects and conducts independent research in support of CINT internal science program.

Normand Modine – (CINT Scientist) Provides support for approved CINT user projects and conducts independent research in support of CINT internal science program.

Mark Stevens - (CINT Scientist) Provides support for approved CINT user projects and conducts independent research in support of CINT internal science program.

Sergei Tretiak – (CINT Scientist) Provides support for approved CINT user projects and conducts independent research in support of CINT internal science program.

Stuart Trugman – (CINT Scientist) Provides support for approved CINT user projects and conducts independent research in support of CINT internal science program.

Jianxin Zhu – (TSNP Partner Science Leader) Provides scientific leadership for Thrust, provides support for approved CINT user projects and conducts independent research in support of CINT internal science program.

B. Other Personnel

Postdoctoral Associates – Conduct research in support of CINT internal science program and work with users as appropriate to support user projects.

G. Other Direct Costs

1. Materials and Supplies –Thrust staff travel costs; publication costs.

11. Description of Facilities and Resources

The TSNP thrust draws on the long established expertise of cutting edge research at SNL and LANL. SNL has long been an international leader in theory, simulation and modeling of molecular systems and interactions. LANL is an established world leader in the field of hard materials and their electronic, magnetic, and optical properties. Theory and modeling at both Sandia and Los Alamos provide a strong background for the TSNP thrust work at CINT.

CINT scientist and users have benefited from being able to run on SNL's institutional computing clusters at no additional cost to the DOE. SNL provided over 63 million-core hours in FY2014 and 101 million-core hours in FY2015 of computing time for CINT projects. Recently we have also succeeded in securing an institutional commitment of computing support at LANL. We expect to complete a transition to LANL institutional computing, while the existing CINT Linux cluster is kept in service during the transition period.