FWP Title: Studies of Nanoscale Structure and Structural Defects in Advanced Materials **Brookhaven National Laboratory**
FWP Number: MA-015-MACA **B&R Code: KC0201010**

Program Abstract:

The goal of this program is to study property sensitive nanoscale structure and defects in technologically-important materials such as superconductors, multiferroics, and other functional materials. Advanced quantitative electron microscopy techniques, such as coherent diffraction, atomic imaging, atomically-resolved spectroscopy, and phase retrieval methods including electron holography are developed and employed to study material behaviors. Computer simulations and theoretical modeling are carried out to aid the interpretation of experimental data. Fabrication of thin films with tailored microstructure and nano-assemblies to understand materials' electronic and magnetic response under applied stimulus is also incorporated.

Program Impact:

The understanding of the structure and property relationship of a complex material entails a wide range of characterization capabilities. The impact of our work is the development of advanced imaging diffraction and spectroscopy instrumentation and methods that can be broadly applied to quantitatively characterize a variety of materials and their behavior at nanoscale. Such development requires significant resources that is suitable for a national lab setting and cannot be achieved by individual university grants. Applications to various model systems and strongly correlated electron oxides including energy related materials are demonstrated.

FY 2009 Authorized Budget (New BA): $1,898K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE (Clearly delineate status of individual: PI, PD, student. Technical Support Staff):

Y. Zhu (PI, 75%), J. Tao (staff, 100%), L. Wu (staff, 100%), V.V. Volkov (staff, 100%), M.A. Schofield (staff, 100%), M.G. Han (postdoc, 70%) and Lei Huang (Ph.D student, 100%,).

Interactions: (limit to current interactions and collaborations)

Internal—Oxide molecular beam epitaxy group (I. Bozovic), Energy materials group (Q. Li, D.O. Welch), Neutron scattering group (J. Tranquada), Synchrotron x-ray diffraction group (J. Hill), Condensed-matter theory group (W. Ku); Center for Functional Nanomaterials (D. Su, E. Sutter, W. Han); Chemistry Fuel-cell group (R.R. Adzic), Battery group (Q. Yang), Catalysis group (J. Hanson, J. Rodriguez), NSLS (D. Fisher, C.C. Kao, A. Frankel), Biology STEM group (J. Wall). External—Princeton University (R. Cava), Columbia University (L. Brus, I. Herman, R. Osgood), Stony Brook University (C. Grey, M. Dudley, K.K. Likharev, M. Rafailovich), Yale University (C.H. Ahn, V.E. Henrich, E.I. Altman), ORNL (S. Pennycook), UC San Diego (I. Schuler), University of Wisconsin at Madison (C.B. Eom), Cornell University (D. Muller), MIT (S. Gradecak, C. Ross), Harvard (D. Bell), Northwestern University (M. Kanatzidis, V. Dravid), General Motors (J. Yang), Washington University at St. Louis (Y. Xia), University of Alberta (R. F. Egerton), Demark Technical University (M. Beleggia), and University of Goettingen (Ch. Jooss) and Hitachi (H. Inada).

FWP Title: Superconducting Materials **Brookhaven National Laboratory**
FWP Number: MA-012-MABA **B&R Code: KC0201030**

Program Abstract:

This program studies the basic relationships between the structure and properties of superconductors to provide understanding of the fundamental materials science and physics required for their energy applications. Superconductors and related materials, which have a wide range of superconducting, magnetic, and other properties, are being made to understand the effect of competing orders, chemical doping, interface, and structure defects on superconducting properties. Both equilibrium and non-equilibrium synthesis routes are used to explore a broad phase space of superconductors and to enhance the properties of superconducting materials. Because they determine the limits to energy applications, the emphasis of this program is on improving the critical temperature T_c, and the critical current density J_c. By exploiting the range of advanced experimental techniques available at Brookhaven National Laboratory, we seek to understand and control the transport properties of superconducting materials by tackling the key science issues, from the macroscopic to the atomic levels. Research activities primarily focused on: (1) the response of superconductivity to competing order parameters, crystal defects, doping, and interface, which could provide new strategies for enhancing T_c and reducing electronic anisotropy, and (2) response and control of superconducting transport properties by defect tuning, where the simultaneous increase of J_c and reduction of the J_c anisotropy ratio can be achieved by tuning the defect structures. This could lead to effective and practical superconductors for highly efficient electricity transmission. Coordinated studies involve synthesis, structural characterization, transport, thermodynamic, and magnetic property characterization.

Program Impact:

This group is synergistic with the other groups at Condensed Matter Physics and Materials Science Department, such as the Electron Spectroscopy Group, Electron Microscopy Group and Neutron Scattering Group. Cross-distribution of key scientific issues is reflected in the collaborative research to probe structure, composition, charge, spin, and crystal structure and defects. Relationship between the structural and transport property obtained in this group is critical to understand the electronic and magnetic structure characterized in other groups. Interactions with the department's high temperature superconductor - Coated Conductor - development programs has results in multiple CRADAs with industrial leaders like American Superconductor Inc. and Superpower, Inc, that depends, directly or indirectly, on the success of this program. Additional connections to investigators at the NSLS and the CFN are made, that resonates with our efforts to probe spectroscopy of complex energy materials that are also being investigated there. The ensemble of interactions above provides a means for this Superconducting Materials Program to respond rapidly and aggressively to new developments. The information this ensemble can access spans vertically from very basic physics and materials questions, through synthesis and structure and property characterization, to finished forms of superconductors that are used in electric utility and other applications.

Number of publications in FY2009: 16; number of invited talks in FY2009: 7.

FY 2009 Authorized Budget (New BA): $714K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE (Clearly delineate status of individual: PI, PD, student. Technical Support Staff):
Qiang Li (PI) – 90%, Weidong Si (Scientific Staff) – 70%, Qing Jie (Ph. D student) –50%, J. Zhou (Ph. D student) – 50%

Interactions: (limit to current interactions and collaborations)

Stanford University, Princeton University, Columbia University, UIUC, Stony Brook University, University of Michigan, ETH-Zurich, AIST-Japan, Livermore National Lab, Oak Ridge National Lab, American Superconductor Inc., Superpower Inc, General Motors Inc.

Related Project URL: (optional)

CRADA between BNL and Superpower Inc. established in 2009 on the development of second-generation high Tc superconducting wires.

FWP Title: Synthesis and Characterization of Individual Carbon and Perovskite Oxide Nanotubes **Brookhaven National Laboratory**
B&R Code: KC0201050
FWP Number: MA-507-MAAA

Program Abstract:

The ability to synthesize, functionalize, and purify nanomaterials and to understand their transport, optical and mechanical properties lies at the forefront of current materials science research. As shown in the DOE report on Basic Research Needs for Solar Energy Utilization, nanostructured materials offer several potential advantages for solar energy conversion by providing relatively high electron and hole transport efficiencies, excitation multiplication possibilities, high surface-to-volume ratios, and short electron-hole diffusion lengths to junctions. Although it is tempting to combine distinct nanomaterial components for solar conversion in order to take advantage of such attractive qualities, the fundamental role of nanoscale heterojunctions in promoting exciton dissociation and charge separation is not understood. It is expected that junctions between low dimensional materials will behave differently than bulk junctions. We will address the important question of the efficiency of charge separation versus recombination or trapping in a prototype heterogeneous nanomaterial systems: 0d-1d nanomaterial hybrids. We also expect to develop an emphasis on understanding metal oxide nanostructures of significance to the solar initiative, based primarily on titanium dioxide. We have the ability to synthesize high quality samples and to study the properties and structure (both electronic and physical) of individual nanomaterial samples, thus eliminating the uncertainties in ensemble averaging over many structures. Working with our theoretical collaborators, these studies will clarify the potential of nanoscale heterojunctions for charge separation in solar electric generation.

In order to achieve our overall goal of evaluating the potential of nanomaterial heterostructures to provide increased overall efficiency for solar electric generation, the components listed above must work closely and well together. For example, the synthesis team must work closely with the characterization team to ensure quality of samples, and to provide the right range of these parameters since our theoretical estimations show that the relative band structures will be important in determining the prospects for optimization of charge separation. The theoreticians must work closely with the experimentalists on interpretation of data and development of an overall model. To accomplish this integration, there are multiple levels of coordination among the researchers.

Program Impact:

Brookhaven National Laboratory (BNL) has established expertise in the synthesis of high-quality and novel nanomaterial systems, and in techniques for the purification, chemical functionalization, and characterization of their composition and structure, including powerful techniques utilizing the National Synchrotron Light Source. Brookhaven has also defined capabilities for characterization of the transport and optical properties of individual quasi-1d wires of nanomaterials and is developing new techniques for the characterization of the structure of the individual nanomaterials. The BNL theory group is building the theoretical foundations to understand these material properties. In this work, we are correlating the chemical nature of nanomaterials with fundamental understanding of charge separation and recombination toward enabling the rational design of functional nanomaterials with enhanced physical properties. Specific recent advances include the synthesis of high quality perovskite metal oxide nanostructures, synthesis of carbon nanotube-quantum dot heterostructures, and spectroscopy of individual carbon nanotubes. The spectroscopy studies have revealed the dependence of electroluminescence on nanotube length and the role of electron-phonon coupling in non-equilibrium carrier relaxation. New studies will examine the role of excitons in carbon nanotube materials, an exploration of the nature of our newly synthesized nanotube-quantum dot heterostructures, and the characterization of electronic properties of classes of individual metal oxide nanowires.

FY 2009 Authorized Budget (New BA): $414K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE (Clearly delineate status of individual: PI, PD, and student. Technical Support Staff):
S.S. Wong (PI - 50%); F. Zhang (student – 100%)

Interactions: (limit to current interactions and collaborations)
National Synchrotron Light Source, State University of New York at Stony Brook, NIST, University of Washington.

FWP: Molecular beam epitaxy and nano-structuring of perovskite oxide materials toward an understanding of strongly correlated systems **Brookhaven National Laboratory**
B&R Code: KC0201050 + KC0202010
FWP Number: MA-509-MACA

Program Abstract:

The mechanism of high-temperature superconductivity (HTS) is arguably the most important open problem in Condensed Matter Physics. Some of the most basic questions - what is the role of dimensionality in the HTS phenomenon, what are the spin and the charge of free carriers, what is the nature of superconducting transition, and which effective interaction causes electron pairing - are still open.

We are using a unique molecular beam epitaxy (MBE) system for atomic-layer ('digital') synthesis of complex oxides to fabricate single-crystal films of cuprates, nickelates, bismuthates, etc., as well as a variety of multilayers and superlattices with atomically perfect interfaces. From these we manufacture heterostructures such as SIN, SIS, and SNS junctions, as well as HTS nanowires, nanorings and nanodots. These unique samples are enabling a series of experiments – either in-house or in collaboration with other leading experimental groups listed below - that were not previously possible. These experiments are hoped to provide clear-cut answers to at least some of the above questions, which would significantly impact research on HTS and more broadly on strongly-correlated materials.

Correlated electron materials, transition-metal oxides and HTS are the main trust of research at the CMPMS Department and a 'grand challenge' of the BES Directorate at BNL. The scope and importance of these problems calls for a coherent attack by a range of techniques, which requires a large-scale, coordinated multi-group effort with concentration of significant technical and personnel resources. Layer-by-layer MBE technique to synthesize perfect films and interfaces and to exploit epitaxial effects, and the identification of essential interactions giving rise to HTS, have been singled out as Priority Research Directions in the recent BES Workshop on Superconductivity.

Program Impact:

The program impact is twofold. First, the group has established itself as the source of the highest-quality HTS films, including multilayer hetero-structures engineered down to a single atomic layer. These unique samples are enabling breakthrough research of few dozen groups at national laboratories and leading universities in US and abroad. Second, our own in-house experiments have brought in several important results such as firm evidence of Giant Proximity Effect, discovery of HTS interface superconductivity, and demonstration of HTS in a single CuO_2 layer.

FY 2009 Authorized Budget (New BA): $1,300K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE

I. Bozovic, PI (100%); Anthony Bollinger PD (100%); O. Pelleg PD (100%).

Interactions:

BNL (Y. Zhu, R. Pindak, H. Zhou, R. Adzic, J. Hill, S. Wilkins), LANL (F. Balakirev, A. Migliori, S. Conradson), ANL (J. Freeland), NHMFL (G. Boebinger, S. Riggs, D. Popovic), LBL (B. Freelon, R. Birgenau), ORNL (S. Pennycook), Harvard (J. Hoffman, N. Litombe, M. Aziz, Mondal), Stanford (A. Kapitulnik, H. Karapetyan, T. Geballe), MIT (R. Ashoori, L. Li, N. Gedik), Urbana (P. Abbamonte, S. Smadici), Cornel (D. Muller, D. Schlom), Berkeley (R. Dynes, S. Cybart), Johns Hopkins (P Armitage), Houston (C. W. Chu), Akron (S. Djordjevic); Miami (J. Clayhold); Simon Fraser, Canada (S. Dodge), EPFL, Switzerland (D. Pavuna, G. Dubuis), PSI, Switzerland (E. Morenzoni, A. Suter, P. Willmot), Konstanz, Germany (J. Demsar), Tuebingen, Germany (R. Kleiner, D. Koelle), Chernogolovka, Russia (V. Gasparov), Belgrade, Serbia (Z. Radovic), Bar Ilan, Israel (Y. Yeshurun, I. Sochnikov, A. Shaulov), Weitzman, Israel (E. Zeldov), Hebrew U., Israel (Y. Yacobi), Yonsei U., Korea (J. H. Kim, T. Hong), NTU Singapore (C. Panagopoulos, J. Pereiro), Tsinghua U., China (Y. Wang, J. Zhang).

FWP Title: Exploratory Materials Synthesis and Characterization **Brookhaven National Laboratory**
FWP Number: PM-016 **B&R Code: KC0201050**

Program Abstract:
Research focus is design, discovery, synthesis and characterization of new and improved condensed matter physics model materials. Since many observables are tensor components, there is strong emphasis on single crystals.
Innovative preparative methods are core strengths of the program. New materials are prepared by variety of crystal growth and materials synthesis methods: arc melting and powder metallurgical techniques, high and low temperature intermetallic, oxide, sulfide or halide flux, chemical vapor transport and deposition. Accurate characterization is another important component; therefore automated physical and chemical characterization methods are essential components of the program. In order to optimize synthesis parameters it is necessary to have continuous feedback of structural and physical properties. Quite often the same methods are used to probe and elucidate details of crystal structure and physical properties via X-ray diffraction, transport, thermodynamic and magnetic measurements of new materials at extreme conditions of low temperatures, high magnetic fields and high pressures. This program also uses high magnetic fields (NHMFL) and synchrotron X ray powder diffraction (NSLS BNL) through user proposal system.

Program Impact:
We are engaged in exploratory synthesis and characterization of new materials (crystals), discovery of new phenomena associated with superconductivity, magnetism and correlated electron behavior. Development of new synthesis methods is integral part of our work. This program includes diverse synthesis and characterization skills. Proximity to synchrotron source (NSLS) and expertise in scattering methods at BNL greatly enhances program impact and scope. Our work greatly influences all other programs through collaborative research on our samples. This program synthesized highest purity heavy fermion materials in the world with residual resistivity in several tens of nanoohmcm at low temperatures, thus enabling some landmark studies of quantum criticality and unconventional superconductivity in heavy fermions. It also synthesized large crystals of materials at quantum critical point suitable for inelastic neutron scattering (eg. $CeCoIn_5$ and $YbRh_2Si_2$), thus securing supply of crystals for national neutron sources (NIST MACS) and providing US researchers with competitive advantage (Broholm, Johns Hopkins University). Number of new materials have been discovered and developed in the recent years such as new Kondo Insulator $FeSb_2$ with highest known thermoelectric power factor, Mn_4FeGe_3, highest known non-oxide material suitable with integration in Si and Ge based semiconducting devices with simultaneous high T_C above room temperature and spin polarization, new quasi 1D superconductor Nb_2Se_3 and others.

FY 2009 Authorized Budget (New BA): $575K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE (Clearly delineate status of individual: PI, PD, student. Technical Support Staff):
C. Petrovic (100%), Rongwei Hu (student – until August 2009) 100%

Interactions: (limit to current interactions and collaborations)
Internal: Instrumentation Division (Warren); NSLS (Frenkel); CMPMSD (Zaliznyak, Valla, Johnson, Li, Bozin, Akrap). External: NHMFL (Choi, Tozer); Urbana (Abbamonte); Akron (Dordevic); Belgrade (Popovic); Johns Hopkins (Broholm, Armitage); Columbia (Uemura, Pasupathy); Brown (Mitrovic); Notre Dame (Eskildsen); Sherbrooke (Taillefer), Toronto (Wei, Julian); Ames (Canfield, Bud'ko, Kogan, Prozorov, Kaminski), Univ. of Tokyo (Nakatsuji), Yonsei Univ. Seoul (Lee); UC Irvine (Fisk); ISIS (Stock); Sao Paolo (Pagliuso); Simon Fraser (Dodge); TRIUMF (Storchak); Northwestern (Ketterson)

Related Project URL: http://www.bnl.gov/cmpmsd/emsc/

FWP Title: Neutron Scattering **Brookhaven National Laboratory**
FWP Number: PO-010 **B&R Code: KC020201**

Program Abstract:
This program is organized around the goal of decoding the mechanism(s) responsible for high-temperature superconductivity, with particular focus on the copper oxides, as well as new systems, such as the iron-based superconductors. The main experimental tool is neutron scattering, with experiments performed at the best facilities in the U.S. and abroad. Problems addressed include: doping of correlated insulators, self-organized spin and charge inhomogeneities (such as stripes), electron-phonon coupling, spin dynamics, quantum magnetism in low-dimensional systems, and the impact of disorder. Growth of suitable single-crystal samples is an essential part of the program, with complementary characterizations performed in collaboration with other Brookhaven groups, especially at the National Synchrotron Light Source. This program has close ties to HYSPEC, an inelastic spectrometer with polarization analysis under construction at the Spallation Neutron Source (SNS); it is also involved with the US-Japan cold-neutron triple-axis spectrometer at the High Flux Isotope Reactor (HFIR), as part of the US-Japan Cooperative Program on Neutron Scattering. The BNL-NIST Alliance involves collaborative efforts at the National Institute of Standards and Technology's Center for Neutron Research.

Program Impact:
Discoveries of charge and spin stripe correlations in cuprate superconductors, and demonstration of a universal spin-fluctuation spectrum, have been possible through a sustained effort, including the time-consuming growth of unique, high-quality single-crystal samples of materials such $La_{2-x}Ba_xCuO_4$ and $Bi_2Sr_2CaCu_2O_{8+\delta}$. Discovery of two-dimensional superconductivity in a three-dimensional, stripe-ordered crystal resulted from close collaboration with other BNL groups. This work has motivated new theoretical concepts, such as the pair-density-wave superconducting state. The crystal-growth effort, besides benefiting collaborating groups by providing samples, has also had synergistic impact on other programs, such as the growth of $Cd_{0.9}Zn_{0.1}Te$ crystals for γ-ray detectors aimed at the needs of the Dept. of Homeland Security. With a critical mass of neutron scattering expertise, the group has provided leadership for the HYSPEC Instrument Development Team (commissioning at SNS in FY11), as well as providing direction for the installation of the US-Japan triple-axis spectrometer on Cold Guide 4 at HFIR.

FY 2009 Authorized Budget (New BA): $2150K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE
PIs: J. M. Tranquada (100%), G. D. Gu (100%), M. Hücker (100%), B. Winn (stationed at ORNL, 100%), G. Y Xu (100%), I. Zaliznyak (90%)
Students: J. S. Wen (60%), Z. J. Xu (100%)
Technical Support Staff: K. Mohanty (professional, 50%), E. Stein (technician, 10%)

Interactions: (limit to current interactions and collaborations)
Internal---Condensed Matter Physics & Materials Science Dept.: X-ray Scattering Group, Advanced Energy Materials Group, Electron Spectroscopy Group, Condensed Matter Theory Group, Oxide MBE Group, Spectroscopic Imaging Group, Institute for Advanced Electron Microscopy; The Center for Emergent Superconductivity (an Energy Frontier Research Center); Chemistry Dept.: P. Khalifah.
US-Japan Cooperative Program on Neutron Scattering
External---K. Yamada, WPI-Advanced Institute for Materials Research, Tohoku University, Japan; H. Yoshizawa, ISSP, U. Tokyo, Japan; S.-H. Lee, U. Virginia; M. v. Zimmermann, HASYLAB, Hamburg, Germany; B. Büchner, IFW, Dresden, Germany; M. Braden, U. Cologne, Germany; D. Reznik, U. Colorado; S. A. Kivelson, Stanford U.; T. G. Perring and C. Stock, ISIS, Rutherford-Appleton Lab., UK; P. M. Gehring, NCNR; L.-P. Regnault, CEA-Grenoble, France; A. Yazdani, Princeton U.; D. Basov, UCSD; S. Wakimoto and M. Matsuda, JAEA, Japan.

Related Project URL: http://neutrons.phy.bnl.gov/

FWP Title: X-ray Scattering **Brookhaven National Laboratory**
FWP Number: PO-011 **B&R Code: KC0202010**

Program Abstract:

The central objective of this program is to carry out basic studies of the structural, electronic and magnetic properties of condensed matter systems using synchrotron-based x-ray scattering techniques. Particular emphasis is placed on electronic and magnetic structure and phase behavior, on collective excitations in solids and on the investigation of surface and interfacial phenomena. The X-ray Scattering Group also develops instrumentation, maintains and operates a beamline at the National Synchrotron Light Source and is involved in the development and use of two sectors at the Advanced Photon Source. Research focuses on strongly correlated electron systems. Major long-term objectives include understanding charge dynamics in these systems – over a wide range of timescales, investigations of the role of inhomgeneities in strongly correlated phenomena and the electronic behavior at surfaces and interfaces. Inelastic x-ray scattering and hard and soft x-ray resonant scattering experiments are carried out in close collaboration with related efforts in CMPMSD and at BNL to address these questions. A new research direction within the group has been initiated to utilize pair distribution function methods to solve the structure of nanoscaled objects and fluctuations as applied to energy-relevant materials. This effort is a subtask of the group.

Program Impact:

The Group's longstanding programs concerned with x-ray resonant phenomena, and inelastic x-ray scattering have been seminal in stimulating related efforts worldwide, and remain among the leading programs in these areas today. Efforts in soft condensed matter led to the creation of a new FWP aimed at understanding nanoscale confinement and the role of self-assembly in soft materials. Work in inelastic x-ray scattering led, with others, to the creation of the IXS-CDT at the APS. Developed a soft x-ray grazing incidence diffraction and imaging chamber. These latter two developments required the use of engineering and large teams of PIs only available at National laboratories and support the DOE-BES mission of developing unique tools to study complex materials. The scientific thrusts are aimed at the grand challenge questions of understanding and controlling the emergent properties of complex materials.

FY 2009 Authorized Budget (New BA): $1,735,000
FWP PO-011 $1,200,000
FWP PO-011 Subtask A $535,000

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE (Clearly delineate status of individual: PI, PD, student. Technical Support Staff):
FWP PO-011: Hill (100%, PI), Wilkins (100%, Associate Scientist), Liu (100%, PD), Tobey (10%, PD), Schoenig (50%, technical support staff), Leonhardt (100%, technical support staff), Rementer (33%, Admin support)

FWP PO-011 Subtask A: Billinge (75%, PI), Bozin (100%, Research Associate)

Interactions: (limit to current interactions and collaborations)
Internal: R. Adzic, I. Bozovic, J. Hanson, M. Huecker, P. Khalifah, G. Gu, W. Lu, C. Petrovic, J. Tao J. Tranquada, X. Wang, Y. Zhu
External: Boothroyd, Cavalleri (U. Oxford), Buchner, Geck (IFW-Dresden), Gog, Casa, Kim (ANL), Nagler, Macdougal (ORNL), McMorrow, Robinson (UCL), LeTacon (MPI-Stuttgart), Krisch (ESRF), Fisher, Devereaux (Stanford U.), Kevan (U. Oregon), J. Mitchell (ANL), M. Kanatzidis (NU)

Related Project URL: (optional)
X-ray Group at Brookhaven: http://www.bnl.gov/cmpmsd/xray/
Billinge Columbia web site: http://www.apam.columbia.edu/fac-bios/billinge/faculty.html

FWP Title: Atomistic Transport Mechanisms in Reversible Complex Metal Hydrides **Brookhaven National Laboratory**
FWP Number: BO-130 **B&R Code: KC0202020**

Program Abstract:

Complex metal hydrides have the potential of satisfying the need for lightweight hydrogen storage materials with capacities and absorption/release kinetics adequate for automotive applications. However, among a large class of hydrogen-rich compounds, only one material – sodium aluminum hydride ($NaAlH_4$) – has shown the reversible release and storage of hydrogen at moderate ambient conditions. Empirically, doping with small amounts of titanium was identified as a key element in achieving reversible hydrogen storage.

This interdisciplinary research program focuses on identifying the mechanisms underlying the facile reaction from the Ti-doped, H-depleted material (NaH, Al) to the H-rich storage compound ($NaAlH_4$), with the goal of deriving from this and similar model systems a general understanding of the atomistic mechanisms of solid-state hydrogen storage. In particular, our research emphasizes the identification of the role of dopants and catalysts, of possible nanometer-scale size-effects, and of reaction pathways in environments other than the conventional solid-gas interface, i.e., effects that are largely unexplored but may be harnessed in future hydrogen storage applications. Close attention is also being paid to newly emerging high-performance materials, such as graphene, and the opportunities afforded by their interaction with hydrogen for energy storage and materials processing.

Program Impact:

Experiments on model system in controlled environments, coupled with ab-initio theory and modeling, have led to a fundamental understanding of the initial stages of hydrogen storage reactions in doped alanates. In particular, our work on Al single crystals has demonstrated that Ti dopants efficiently catalyze the dissociation of molecular H_2 to atomic H, which in turn combines with Al atoms to form highly mobile alane species. This process should operate for all alanates. Yet, in practice very few complex hydrides can be hydrogenated reversibly, i.e., the crucial step suppressing hydrogenation in storage materials such as $LiAlH_4$ (10.6 wt.% H) or AlH_3 (10.1 wt.% H) clearly lies in the further reaction of alanes, e.g., with cationic hydride species (LiH) to form a hydrogen-rich compound.

This insight has led to the recognition that pathways other than the conventional solid-state reaction of alane + MH (M: alkali metal) may enable the hydrogenation of a large family of alanate hydrogen storage materials. Experiments on liquid-phase hydrogenation, performed by our team, have confirmed this prediction by demonstrating the first successful formation of several 'irreversible' hydrides, including $LiAlH_4$ and AlH_3. Hence, our work has established a novel synthetic approach to the formation of high-capacity hydrogen storage compounds.

FY 2009 Authorized Budget (New BA): $700K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE (Clearly delineate status of individual: PI, PD, student. Technical Support Staff):
Peter Sutter, BNL (PI; 25 % FTE); James Muckerman, BNL (Co-PI; 12 % FTE); Jason Graetz (Co-PI; 25 % FTE); Altaf Karmi, BNL (Postdoc; 100 % FTE); David Lacina, BNL (Postdoc; 100 % FTE since October 2009); Abdullah Al-Mahboob, BNL (Postdoc, 100 % FTE since September 2009), Yves Chabal, University of Texas-Dallas (Collaborator, contract), Cristian Ciobanu, Colorado School of Mines (Collaborator, contract).

Interactions: (limit to current interactions and collaborations)
Yves Chabal, University of Texas - Dallas; Cristian Ciobanu, Colorado School of Mines; BNL-Center for Functional Nanomaterials; BNL- Chemistry; BNL Materials Science & Condensed Matter Physics.

Related Project URL: (optional)

N/A

FWP Title: PECASE - Chemical and Electrical Energy Storage **Brookhaven National Laboratory**
FWP Number: EST-444-NEDA **B&R Code: KC0202020**

Program Abstract:

The objective of this project is to develop a fundamental understanding of energy storage materials, specifically electrodes for lithium batteries and metal hydrides for hydrogen storage. This includes an investigation of the role of nanostructure on the fundamental electrochemical properties of lithium electrodes. The high surface area and short diffusion paths in these materials ensure fast kinetics and the rapid lattice relaxation and the absence of dislocations are expected to mitigate microstructural cycling damage. Nanoscale electrode materials are synthesized via wet chemical techniques along with physical and chemical deposition. Electrochemistry and electron microscopy is being used to investigate how capacity fade and cycling rate are affected by electrode morphology and microstructure.

The second thrust will focus on developing new approaches to form aluminum hydride (AlH_3). Direct hydrogenation of Al metal requires extremely high pressures and temperatures. However, it is well known that Al readily forms molecular AlHx in the presence of atomic H and disassociation of H2 occurs on Al in the presence of a transition metal. In this thrust I will investigate the possibility of stabilizing alane using electron donors such as amines and also explore the possibility of separating the alane adduct to recover AlH3.

Program Impact:

The increase in energy generated from intermittent, renewable sources and the growing need for mobile energy requires new, efficient means of storing energy. The United States imports nearly 60% of the roughly 20 million barrels per day of total oil consumed. In 2002, consumption of oil for transportation alone was nearly double the level of domestic production. Substantial technological advancements will be necessary to support our future energy storage needs. Specifically, a change toward alternative transportation, such as hybrid electric vehicles, plug-in hybrid-electric vehicles and electric vehicles, is essential for reducing oil dependency.

In this effort we will develop a better molecular and atomic-level understanding of high energy density materials and the physical and chemical processes that occur at interfaces, surfaces and in bulk materials during cycling. The program impact is the development of improved energy storage materials and systems with high energy densities, fast cycling rates and long cycling lifetimes in efficient, economical and safe media.

FY 2009 Authorized Budget (New BA): **FY09 - $50k**
FY10 - $50k

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE (Clearly delineate status of individual: PI, PD, student. Technical Support Staff):
PI: Jason Graetz, 15% FTE

Interactions: (limit to current interactions and collaborations)
Clare Grey (Stony Brook University and Cambridge)
Glenn Amatucci (Rutgers University)
Stan Whittingham (U. of Binghamton)
Shirley Meng (U. San Diego)

FWP Title: Spectroscopic Imaging STM for Complex Electronic Matter Studies **Brookhaven National Laboratory**
FWP Number: PM-007 **B&R Code: KC0202020**

Program Abstract:
Our program consists of : (i) spectroscopic imaging STM (SI-STM) studies of the electronic structure of ***cuprates*** designed to aid in the identification of the mechanism of high temperature superconductivity therein, (ii) SI-STM studies of the newly discovered high temperature superconducting ***ferropnictides*** designed to aid in the identification of the mechanism of high temperature superconductivity therein, (iii) SI-STM studies of electronic nematic states, especially in the ***ruthenates*** and, (iv) SI-STM studies of the mechanism of heavy fermion electronic structure in ***intermetallic*** metals.

Program Impact:
Program has contributed significantly to the application of scanning inelastic spectroscopy to the study of strongly correlated materials. Strong research interactions and collaborations at BNL include:
- Dr. A. Tsvelik (electronic nematicity in ferropnictides)
- Dr. P. Johnson (comparison of photoemission and STM)
- Dr. Genda Gu (studies of cuprates and ferropnictides)
- Dr. J. Tranquada (comparison of neutron scattering and STM)

FY 2009 Authorized Budget (New BA): $410K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE (Clearly delineate status of individual: PI, PD, student. Technical Support Staff):

PI	J.C. Séamus Davis 40%
PI	Jinho Lee 100%
CU Postdoc (Subcontract)	Kazuhiro Fujita 100%
CU Postdoc (Subcontract)	Jhinhwan Lee 100%
CU Grad Student (Subcontract)	Andrew Schmidt 100%
CU Grad Student (Subcontract)	Chung Koo Kim 100%

Interactions:
Interacting Collaborators:
- Dr. M. Norman, ANL, USA
- Dr. Y. Kohsaka and Prof. H. Takagi, RIKEN, Tokyo, Japan
- Dr. P. Wahl, MPI Stuttgart, Germany
- Dr. F. Meyer, Hamburg University, Hamburg, Germany
- Prof. K. McElroy, U of Colorado, USA
- Dr. H. Eisaki, AIST, Tsukuba, Japan
- Prof. S. Uchida, U of Tokyo, Japan.
- Prof. D.-H. Lee and J. Orenstein, U of California, Berkeley, USA
- Dr. M. Yamashita, U of Kyoto, Kyoto, Japan
- Dr. A. Balatsky , LANL, New Mexico, USA
- Dr. M. P. Allan, Prof. F. Baumberger and Prof. A.P. Mackenzie, St. Andrews University, Scotland
- Prof. S.A. Grigera, UNLP, La Plata, Argentina.
- Dr. T.-M. Chuang and Prof. G. Boebinger, NHMFL, U of Florida, Tallahassee, USA
- Drs. S.L. Bud'ko and P. Canfield, AMES Lab, Iowa, USA
- Prof. Graeme Luke, McMaster University, Hamilton, Canada.

Public Interactions: Forty three public presentations were made by the PI during this period including: 1 Prize Lecture, 3 Plenary Lectures, 8 Public Lectures, 13 Invited Lectures at international conferences and 18 Colloquia, 10 of which were international.

Related Project URL: http://www.bnl.gov/cmpmsd/ ; http://people.ccmr.cornell.edu/~jcdavis/ ;

FWP Title: Complexity from Simplicity: Quantum Criticality And Novel Collective Phases in Itinerant Ferromagnets **Brookhaven National Laboratory**
B&R Code: KC0202020
FWP Number: PM-009

Program Abstract:
This project seeks to explicate the essential conditions under which magnetic order is possible, and the range of novel phenomena which occur when order is on the brink of instability, i.e occuring at zero temperature. These quantum critical phenomena are responsible for the functionality of many diffferent classes of advanced materials, and are examples of emergent behavior which results from complex and incompletely understood interactions among the mobile electrons in metals. The goal of this research project is to explore how minimal of a system is required to sustain these complex, many body states, and to determine whether even simple transition metal ferromagnets can host novel critical states, particularly superconductivity. The research we propose combines developing new synthetic infrastructure and approaches for these novel materials and the implementation of advanced measurement techniques, with extensive utilization of national research facilities. The training of students and postdocs is an integral goal of this research project, enabling the next generation of materials-inspired researchers.

Program Impact: The development and exploration of new materials is intrinsically an endeavor which benefits from the formation of an interdisciplinary group which combines both materials synthesis experts and experts in advanced characterization techniques. Few universities have this degree of focus, or the wealth of measurement facilities which the national laboratories can bring to bear on materials classes of the highest interest and importance. This FWP plays both roles. We are well integrated in the BNL effort in the CFN and in CMPMSD to synthesize new nanoscaled systems, both magnetic and superconducting, by providing high quality magnetic characterization as well as small angle x-ray and neutron scattering expertise, as well as diffraction and inelastic neutron scattering measurements. As indicated in the abstract above, we are also engaged in developing new transition metal compounds which are located near quantum critical points. The examples of the cuprates and now the iron-pnictide compounds suggests that such materials can be the precursors for new families of superconductors, and the goal of our FWP is to identify new superconducting classes which can improve on these existing compounds. These materials will be of great interest to others in CMPMSD who have expertise in measurements such as photoemission, x-ray scattering, and neutron scattering, as well as engaging the theorists with developing phenomenologies which will help the synthesis effort determine the most promising new directions. Having all this expertise metaphorically under one roof is expected to greatly increase the speed with which BNL can characterize and then optimize the superconducting properties of these materials, so the judgment can be made as to their technological futures.

FY 2009 Authorized Budget (New BA): $550K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE (Clearly delineate status of individual: PI, PD, student. Technical Support Staff):
M. C. Aronson 50% FTE PI
M. Feygenson 100% FTE, PD
L. Peragine 15% FTE, Support
K. Mohanty 2% FTE, Support
K. Sutter 6% FTE, Support

Interactions: (limit to current interactions and collaborations)
BNL/CFN: W. Han, O. Gang, Y. Zhu, A. Tkachenko
BNL/Chemistry: P. Khalifah
BNL/CMPMSD: S. Wong, G. Gu, A. Tsvelik, V. Solovyov, Y. Zhu
BNL/NSLS: K. Nelson, L. Yang
Stony Brook University: J. Parise, P. Khalifah, M. Dawber
Rutgers University: G. Kotliar, P. Coleman, P. Chandra
University of Michigan: J. W. Allen
University of New Hampshire: X. Teng
University of California-San Diego: D. Basov, M. B. Maple
University of California-Irvine: Z. Fisk
University of California-Riverside: D. MacLaughlin
Louisiana State University: J. Chan
Oak Ridge National Laboratory: V. Urban, M. Hagen, S. Nagler
NCNR/NIST: J. Lynn, J. Borchers

FWP Title: Electron Spectroscopy **Brookhaven National Laboratory**
FWP Number: PO-016 **B&R Code: KC0202020**

Program Abstract:

The Electron Spectroscopy Group's primary focus is on the electronic structure and dynamics of condensed matter systems. The group carries out studies on a range of materials including strongly correlated systems and thin metallic films. A special emphasis is placed on studies of High Tc and related materials. The primary techniques used include High-Resolution Photoemission and Infra-Red Spectroscopy or Optical Conductivity. The experiments are carried out both within the laboratories in the Condensed Matter Physics and Materials Science Department and at the National Synchrotron Light Source. The emphasis is on the study of the low energy excitations and the nature of the interactions of the latter with their environment. The group has also established a successful pulsed laser deposition facility for the study of thin films.

Program Impact:

That the group has had a major impact in characterizing the electronic structure of correlated systems as evidenced by the large number of citations and by the number of invited talks at major international and national conferences. The program has established one of the leading spectroscopy groups in the world working in the area of strongly-correlated electrons. In particular the group, using the techniques, photoelectron spectroscopy and optical conductivity, has had a major impact in the areas of high Tc superconductivity, magnetic thin films and multilayers and surfaces. The group has demonstrated a scaling law relating the superfluid density to the product of the normal state conductivity and the superconducting transition temperature for the high Tc superconducting cuprates, and pioneered methods of extracting self-energy effects from photoemission spectra. The group was the first to identify the kink or mass renormalization observed in the nodal direction of the high Tc materials. Further the group has introduced the method of analysis in photoemission involving Momentum Distribution Curves (MDC). More recently still using new methods of analysis the group has identified a particle-hole asymmetry in the cuprates, indicative of the presence of Fermi hole pockets.

FY 2009 Authorized Budget (New BA): $1650K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE

PI's: Peter D. Johnson (Group Leader, 25%); Christopher Homes (100%), Tonica Valla (90%), Zhihui Pan (P.D. 50%), Hongbo Yang (P.D. 80%), A. Akrap (P.D. 80%) Student: J. Rameau (100%)
Technical Support Staff: Fran Loeb (100%), Al Langhorn (100%), Weidong Si (30%)

Interactions: (limit to current interactions and collaborations)

A.Tsvelik, G.D. Gu, Qiang Li, M. Hücker, J.M. Tranquada, I. Zaliznyak, L. Zhang, J. Camacho
W. Ku, M. Khodas, A. Gozar, CMPMSD, BNL
R. Osgood, A. Millis, Columbia University
T.M. Rice, ETH Zurich
F. Zhang, University of Hong Kong
R.P.S.M. Lobo, LPM/ESPCI/CNRS/UPMC Paris;
D.N. Basov, UCSD
D. Broun, W. Huttema, Simon Fraser University, Canada
P. Canfield, S. Bud'ko, A. Kaminski, Ames, Iowa
A. Chubukov, UW-Madison
J. Carbotte, McMaster University, Canada;
A. Fedorov, LBL
A. C. Walters, C. A. Howard, M. Ellerby, University College, London
P. Pervan, M. Milun, M. Kralj, I. Pletikosic, Institute of Physics, Zagreb

Related Project URL: http://infrared.phy.bnl.gov/

FWP Title: Electronic Properties of Transition-Metal-Compound Nanotubes **Brookhaven National Laboratory**
FWP Number: PM-002 **B&R Code: KC0202030**

Program Abstract:

This program is directed on first-principles theoretical studies of electronic structure and excitation properties of several classes of transition-metal-compound nanotubes and nanoheterostructures that are of great scientific and technical interest. In addition, pronounced nano-scale physics in strongly correlated bulk materials are of great interest, with a focus on the potential modulation of these already interesting and important properties in nano-scale systems. Beside the conventional first-principles methods, the study also includes new theoretical development to properly account for the strong many-body interactions and short-range order essential to the rich correlated nature of these materials. The goal of this research is to bring the scientific research field closer toward a broader and deeper understanding of electron correlations in these materials, thus guiding the discovery and design of new functional nanomaterials, especially for applications in solar energy, thermoelectricity, and superconductivity, all of which are essential to the central missions of DOE-BES and BNL. These efforts respond to the DOE initiative in Theoretical Nanoscience and the activity at BNL's Center for Functional Nanomaterials (CFN) and the National Synchrotron Light Source (NSLS).

Program Impact:

A simultaneous handling of the material specific complexity and the strong many-body interaction in the transition metal compounds renders the targeted families of material far beyond the reach of traditional first-principles theoretical methods. This program gathered researchers of different expertise to develop technically advanced first-principles theoretical/computational tools designed to address the important and rich energy-applications related properties of these materials. The necessity of combining such a wide range of expertise (density functional theory, many-body perturbation theory, exact diagonalization and numerical canonical transformation) is obvious for such a challenging problem. In addition, the theoretical advancement benefit greatly from the strong interplay between the theory and the various experiments conducted in Brookhaven and other DOE light sources, both in supporting the experimental discoveries, and in using the state-of-the-art experimental data to benchmark and refinement of the new theory.

FY 2009 Authorized Budget (New BA): $410K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE (Clearly delineate status of individual: PI, PD, student. Technical Support Staff):
PI: W. Ku (10%), W. Yin (100%), S. White (UCI, 10%)
PD: C. Lee (40%), W. Garber (50%), Y. Yildirim (100%)
Student: T. Berlijn (100%)

Interactions: (limit to current interactions and collaborations)
W. Ku, C. Lee, G. Xu, and J. Tranquada (Neutron Scattering), W. Ku, T. Berlijn, and T. Valla (Electron Spectroscopy), W. Ku, C. Lee, and I. Zaliznyak (Neutron Scattering), W. Ku, C. Lee, S. Billinge and J. Hill (X-ray Scattering), W. Ku and Y. Zhu (Electron Microscopy), W. Ku, W. Yin, and D. Mattis (Univ. of Utah)

FWP Title: Condensed Matter Theory **Brookhaven National Laboratory**
FWP Number: PO-015 **B&R Code: KC0202030**

Program Abstract:

The program is directed on a study of strongly correlated and complex systems. The two major research directions present in the group are in the areas of Strongly Correlated Systems (SCS) and Complex Nanoscale Networks (CNN). These directions are closely tied to ongoing experimental efforts at Brookhaven National Laboratory.

SCS are defined as systems whose behavior is determined by collective phenomena and therefore cannot be adiabatically traced back to the behavior of noninteracting particles. The best known examples of SCS include doped Mott insulators (such as the cuprates), quasi-one-dimensional systems and electron systems in the Fractional Quantum Hall regime. Theoretical study of SCS requires non-perturbative methods which, at the present time are well developed only for strictly one-dimensional systems. Therefore our number one priority is a generalization of these methods beyond their present area of application. To this end we have developed a numerical renormalization group technology able to study the spectrum and correlation functions of arbitrary continuum one dimensional systems together with the spectrum of two dimensional arrays of coupled one dimensional chains. As a particular application of this methodology, we are studying the many-body spectrum of gapped carbon nanotubes.

To incorporate the realistic complexity of real SCS materials, we are also developing novel first-principles numerical methods, including a Wannier function-based many-body down-folding approach that reduce the energy of first-principles Hamiltonian from 20eV scale to 1eV. In particular, the focus has been on the local quasi-particle and charge excitations in strongly interacting charge transfer insulators. This method has been applied to the cuprates and other transition metal oxides.

In the area of Complex Nanoscale Networks, we focus upon both the understanding of nanoparticle systems with a continuing effort in large-scale computational modeling of biological systems such as biomolecular networks operating inside living cells. This work is carried out in collaboration with Alexei Tkachenko from BNL's Center for Functional Nanomaterials and Bill Studier from BNL's Biology Department.

Program Impact:

The results achieved have come as the fruit of extended collaborations involving various experimental and theoretical groups inside and outside BNL. Intra-BNL collaborations include CMPMS, Physics, CFN, NSLS, and Biology departments.

The group's work on complex mass-action dynamics is closely related to the theoretical (A. Tkachenko) and experimental (O. Gang) research carried out within the BNL Center for Functional Nanomaterials.

FY 2009 Authorized Budget (New BA): $1,450K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE (Clearly delineate status of individual: PI, PD, student. Technical Support Staff):
PI: A. M. Tsvelik 100%, S. Maslov 100%, R. M. Konik 100%, Wei Ku 90%
Technical Support Staff:

Interactions: (limit to current interactions and collaborations)
A. Tsvelik, R. Konik, and T. M. Rice (supported by CES), A. Tsvelik and P. D. Johnson, H. Yang (Electron Spectroscopy), A. Tsvelik, M. Khodas and I. Zaliznyak (Neutron Scattering), T. Valla, (Electron Spectroscopy) A. Tsvelik and M. Khodas (postdoc supported by LDRD), A. Tsvelik and R. Pisarski, L. McLerran (Nuclear Physics), A. Tsvelik, R. Konik and F. H. L. Essler (Oxford), A. Tsvelik, R. Konik and G. Shlyapnikov (Orsay), R. Konik and J.-S. Caux (Amsterdam), R. Konik and G. Mussardo (Sissa, Trieste), W. Ku, G. Xu, and J. Tranquada (Neutron Scattering), W. Ku and T. Valla (Electron Spectroscopy), W. Ku and I. Zaliznyak (Neutron Scattering), W. Ku, S. Billinge and J. Hill (X-ray Scattering), W. Ku and Y. Zhu (Electron Microscopy), W. Ku and K. Knizek (Institute of Physics ASCR,Czech), S. Maslov and A. Tkachenko (CFN), S. Maslov and O. Gang (CFN), S. Maslov and B. Studier (BNL Biology). S. Maslov and K. Sneppen (Copenhagen), S. Maslov and S. Redner (Boston U.)

FWP Title: Biology-inspired programmable assembly of functional nano-structures
FWP Number: MA-114-MAEA

Brookhaven National Laboratory
B&R Code: KC0203010

Program Abstract:

There is a great demand for developing approaches for a large scale assembly with nanometer precision. Our approach utilizes a strategy of a bio-programmable assembly, in which biomolecules with highly selective interactions, like DNA and proteins, guide an assembly of inorganic nano-components. The main approaches are based on (i) adopting the addressable, "key-lock" interactions of biomolecules to nano-environments; (ii) understanding and incorporation of diverse physical interactions, entropic effects, and energetic landscapes of biomolecules; (iii) and developing methods for tailoring biomolecular structures. Our research strategy combines the development of methods for the assembly of nano-architectures with exploration of their microscopic structures using electron and atomic force microscopies, x-ray and light scattering, and optical spectroscopy.

Program Impact:

The well established progress of this proposal is based on synergetic expertise of PIs in physical and biological aspects of self-assembly. One of PIs (Gang) provides a strong expertise in soft matter physics and in-situ characterization of hybrid systems, while the second PI (van der Lelie) provides expertise in biomolecular methods and their application to nanomaterials. Additionally, the close proximity of such BNL user facilities as NSLS and CFN allows to tremendously speed up characterization studies using x-ray scattering, optical and electron microscopy.

FY 2009 Authorized Budget (New BA): $345k

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE (Clearly delineate status of individual: PI, PD, student. Technical Support Staff):
Oleg Gang (PI), 25%
Daniel van der Lelie (PI), 10 %
Huimimg Xiong, Post Doc, 100%
Fang Lu, Post Doc, 100 %
Yian-Biao Zhang, technical support staff, 10 %

Interactions: (limit to current interactions and collaborations)

We have established and continue the development of a broad range of collaboration related to structural behavior and functionality of bio-assembled nano-systems. Our collaborations are focused on: optical properties of assemblies with Matt Sfeir (BNL); kinetics and dynamics of bio-assembled structures with Dmytro Nykypanchuk (BNL) and Mathew May (Syracuse Univ.); the behavior of nano-objects at charged liquid interfaces with Masa Fukuto (BNL) and Lin Yang (BNL); approaches for a fabrication of precisely designed nano-object with nucleic acids with Alex Kotlyar (Tel-Aviv University); a theoretical understanding of assembly phase behavior on microscopic level with Sharon Glotzer (Univ. Michigan) and Alexei Tkachenko (BNL); a protein driven assembly with Hiroshi Matsui (Hunter College) and Paul Freimuth (BNL); magnetic properties of engineered particles clusters with Magee Aronson (Stony Brook University-BNL); a shape-induced phase behavior of particles assemblies with Stephanie Vial (International Iberian Nanotechnolgoy Lab) and Yugang Zhang (CAS).

FWP Title: — Nanotemplate Directed Assembly of Soft-Matter and Biomolecular Materials **Brookhaven National Laboratory**
B&R Code: KC0203010
FWP Number: PO-034

Program Abstract:
The primary goal of the group is to understand the effects of nanoscale confinement and the role of self-assembly in soft materials through the use of patterned templates and well-defined interfaces. We use synchrotron x-ray scattering, scanning probe and optical microscopy techniques to study fundamental properties of complex simple liquids, macromolecular assemblies, polymers, and biomolecular materials. The challenges are (1) to understand liquids under nano-confinement, (2) how templates and confinement can be used to direct the assembly of biomolecular materials, nanoparticles and diblock copolymer thin films, (3) to understand the fundamental interactions which give rise to similar self-assembly behaviour for a wide variety of systems, (4) how the order correlates with function. Understanding structural aspects of self-assembly and thin organic films underlies many emerging organic based devices and energy technologies.

Program Impact:
The Group has pioneered a variety of synchrotron techniques, including surface x-ray scattering, to investigate the structure and phase behavior of complex liquid interfaces, including more recently those on nanopatterned surfaces. The Group has led the development of liquid surface x-ray scattering both at the NSLS and the APS. The group has also pioneered the use of environmental non-contact AFM for the study of nanoscale liquid interfaces. The group has demonstrated the important role that nanopatterned surfaces and templates play in controlling the behavior of liquid, and biomolecular materials and polymer film assembly. Our studies confirm long-standing theoretical prediction on the effects of the shape and size of nanodrops and how liquids fill nanotexture surfaces. Work at buried liquid interfaces is helping to provide a structural basis for a wide array of interdisciplinary problems ranging from protein crystallization to molecular electronics. The Group is well know for its discovery of surface freezing in alkanes and has recently shown that similar equilibrium surface freezing also occurs at solid interfaces.

FY 2009 Authorized Budget (New BA): $930K

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE (Clearly delineate status of individual: PI, PD, student. Technical Support Staff):
Ben Ocko (PI:90%), Masa Fukuto(coPI:100%), Antonio Checco (coPI:90%),Tommy Hoffman (PD:70%), Sumit Kewalramani (PD:10%), Htay Hlaing (student:50%)

Interactions: (limit to current interactions and collaborations)
The researchers in the group have significant scientific overlap and interactions with scientist at the National Synchrotron Light Source and the Center for Functional Nanomaterials and with university collaborators. Masa Fukuto collaborates with Lin Yang (NSLS), Oleg Gang (CFN) and Qian Wang (Univ. S. Carolina) to investigate biomolecular and inorganic nanoparticle assembly at liquid interfaces. Antonio Checco and Ben Ocko are working with members of the Environmental Sciences group to investigate the deliquisence of salt nano-crystals using non-contact AFM. Antonio Checco and Ben Ocko are working with Tom Russell's Group (Univ. Mass) to use our AFM based chemical nanopatterns to template the self-assembly of block copolymer thin films. Ben Ocko collaborates with Liz Dobiz (Hitachi) and Siegfried Dietrich (Max Planck) to investigate the wetting of nanostructured interfaces. Ben Ocko has a long-standing collaboration with Moshe Deutsch (Bar Ilan University) to study surface freezing. Antonio Checco and Ben Ocko are collaborating with Charles Black (CFN) and Elaine DiMasi (NSLS) to investigate nanoscale aspects of superhydrophobicity. The group is working closely with Charles Black and Robert Grubbs(CFN), supported by a BNL Energy LDRD, to develop new approaches to improve the performance of organic photovoltaic devices. The Group is a member of the Liquid Spectrometer Partner User Proposal at the Advanced Photon Source.

Related Project URL: http://www.bnl.gov/cmpmsd/softmatter/