

NHMFL for research and/or student training. The approved proposals covered nine different projects which have been under way during the past year and are described separately by the campus investigators in this Annual Report. Access to the NHMFL provides unparalleled opportunities to work with the highest magnetic fields. For example, the UCDRD program arranged for Vojislav Srdanov (UC Santa Barbara) and his student, Andrew Saab, to participate in very unique explosive flux compression shots that Los Alamos carries out jointly with Russian scientists. Thus, these highly specialized, world-record experiments, which reach 850 tesla and have been occurring annually at Los Alamos with NHMFL co-sponsorship, now also have university involvement. Apart from the access to the NHMFL, these projects also provide other benefits to the users and to Los Alamos. Two of the proposals, an experimental project proposed by Hongwen Jiang (UC Los Angeles) and a theoretical project proposed by Dung-Hai Lee (UC Berkeley) complimented each other by addressing the same subject, the quantum Hall effect. Their involvement with the NHMFL initiated a collaboration between them. As a result of another project, proposed by David Awschalom (UC Santa Barbara), Los Alamos was able to recruit an outstanding graduate in the area of time-resolved spectroscopy into a Director's Postdoctoral Fellow position for the NHMFL. At least one graduate student, Alex Yatskar, working with Ward Beyermann (UC Riverside) accomplished his Ph.D. research at NHMFL through this UCDRD program and another, Robert Dickey, working with Brian Maple (UC San Diego) at the NHMFL, has nearly finished his PhD research. All of the UCDRD-supported researchers profited technically from the availability of the new NHMFL tools for high field research. They also profited because they became involved at an early stage. This should help them in securing other grants to exploit these tools. The NHMFL continues to provide new technical opportunities. As an example, the next major NHMFL magnet, a 60 tesla quasi-continuous magnet, the

most powerful of its class in the world, is undergoing final commissioning and will be available to users in early 1998.

Descriptions of individual projects carried out under this program are provided separately in this report by the investigators of these projects.

## **9744(2) Research and Education Utilizing the NHMFL: Physics of Quantum Hall Devices in Ultra-High Magnetic Fields**

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### **Abstract**

Strong magnetic fields are a powerful tool for studying physical properties of low-dimensional semiconductor structures. The pulsed magnet facilities at the Los Alamos National High Magnetic Field Laboratory (NHMFL) have provided an unique opportunity to explore new correlated electronic phases of quantum Hall devices in ultra-high magnetic fields. We have performed both magneto-transport and photoluminescence experiments in the pulsed magnet for fields up to 50 T and temperatures down to 500 mK to study several types of GaAs/AlGaAs heterostructures. The findings of our exploratory experiments are summarized below.

By using the magneto-optics setup at the NHMFL we have studied the photoluminescence spectra in the under-explored Hall insulator phase. We found that the band-edge emission peak splits into two separated peaks in the high fields. Our observations provide evidence that the dissipationless quantum Hall liquids are separated by regions containing localized normal electrons in the Hall insulator phase. This finding also gives further experimental support of the view of charge-flux duality in the quantum Hall effect.

By using a heterostructure containing dense electron gas we have studied many-body photoluminescence spectra around the fully filled lowest Landau level. We have found that the conventional band-edge emission peak terminates abruptly at a magnetic field of about 30 T, and is followed by the appearance of a new peak at an energy position of 10 meV below that given by the normal ones. We believe this anomalous high-field effect is due to a magnetic-field-induced phase transition of photo-excited holes from a free state to a spatially localized state due to the many-body interactions.

We have also used the pulsed field to characterize a new type of semiconductor structure grown by molecular beam epitaxy at low temperature. This type of structure has new device potential. By analyzing the magneto-resistance oscillations in the transport data, we found that there are as many as five quantum sub-band levels occupied in this very high density ( $\sim 10^{13}/\text{cm}^2$ ) heterostructure. This exploratory research has given the collaborators at UC Los Angeles a head start in utilizing the unique ultra-high magnetic field facilities at LANL for research involving low-dimensional semiconductor structures. The findings are not only important to the basic understanding of electron-photon interaction in low-dimensional systems, but are also useful in the efficient design of heterostructure devices.

## Refereed Publications

1. X. Y. Lee, H.W. Jiang, Y. Kim, and W.J. Schaff, "Anomalous Photoluminescence Spectrum in High Magnetic Fields: Evidence of Hole Localization in a GaAs/AlGaAs Heterostructure," *Phys. Rev. Lett.* (submitted).

## Non-Refereed Publications

1. H.W. Jiang, X.Y. Lee, Y. Kim, and W.J. Schaff, "Studies of High-Field Fermi-Edge-Induced Magnetoluminescence in Pulsed Magnets," *National High Magnetic Field Laboratory 1997 Annual Report*, 1, 121 (1997).
2. H.W. Jiang, X.Y. Lee, Y. Kim, and W.J. Schaff, "Magnetotransport Characterization of a Low-Temperature-Grown GaAs Heterostructure in Pulsed Fields," *National High Magnetic Field Laboratory 1997 Annual Report*, 1, 124 (1997).
3. X.Y. Lee, Y.M. Kim, H.W. Jiang, W.J. Schaff, "Studies of High-Field Fermi-Edge-Induced Magnetoluminescence in Pulsed Magnets," *American Physical Society Bulletin*, 43, 105 (1997).

## Presentation

1. X.Y. Lee, Y.M. Kim, H.W. Jiang, W.J. Schaff, "Studies of High-Field Fermi-Edge-Induced Magnetoluminescence in Pulsed Magnets," *American Physical Society Annual Meeting*, Los Angeles, CA, March 16-20, 1997 (contributed).

### **9744(3) Research and Education Utilizing the NHMFL: Experiments at the NHMFL at the Los Alamos National Laboratory During Winter 1997**

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#### **Abstract**

Experiments were carried out at the National High Magnetic Field Laboratory on the compound  $\text{BaVS}_3$ . This compound exhibits a metal-insulator (MI) transition at  $T_{mi} = 70\text{K}$  from a high temperature metallic paramagnetic state to a low temperature non-magnetic insulating state. The purpose of the experiments was to learn more about the nature of the magnetism, which is poorly understood. Specifically, would electron correlations which are responsible for the MI transition promote local moment magnetism? The study of such correlations is of interest to the Los Alamos National Laboratory and to the Department of Energy because such correlations play a key role in the behavior of actinide compounds and high temperature superconductors.

We measured the magnetization of  $\text{BaVS}_3$  powders in pulsed fields for  $0 < B < 45\text{T}$  and found that the magnetization is a linear function of  $B$  at all temperatures; in particular, there is no indication of a field induced transition for  $T < T_{mi}$ . We measured the magnetoresistance of a single crystal of  $\text{BaVS}_3$  at a number of fixed temperatures as a function of (continuous) field  $B_{\perp}$  applied perpendicular to the current, which flowed

along the needle axis (the  $c$ -axis of the single crystals). We found that the magnetoresistance is negative for  $T < T_{mi}$  and  $B_{\perp} < 20\text{T}$  and is of approximate magnitude  $[\Delta\rho/\rho_0]/B \sim 1\%/\text{T}$ ; for  $T > T_{mi}$  the magnetoresistance is vanishingly small. The negative magnetoresistance in the insulating state suggests that the magnetic field promotes metallic behavior; for sufficiently large field we expect a transition into the metallic state. However, the linearity of the magnetization suggests that such a transition does not occur for  $B < 45\text{T}$ . Efforts to measure the magnetoresistance in the pulsed field magnet were not successful: It is not possible to attain the high level of thermal stability during the pulse necessary to give an accurate measurement of  $\rho(B)$  in the presence of the large temperature derivative  $d\rho/dT$  in the insulating state. Future plans are to measure the magnetoresistance for field  $B_{\parallel}$  parallel to the  $c$ -axis.

The significance of these results is that the magnetic field has only a minor effect on the transition from the metallic to the insulating state; this means that electron correlations that are responsible for the MI transition do not promote local moment magnetism. This research program strengthens an existing collaboration between UC Irvine and the Condensed Matter Physics Group at LANL, and hence promotes publicly stated goals of both institutions.

### **9744(4) Research and Education Utilizing the NHMFL: The Physics of Two-Dimensional Electron Gas at Filling Factor 1/2**

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## Abstract

Thanks to over fifteen years' research, a global understanding of the phase structure of a two-dimensional electron gas (2DEG) under high magnetic field is gradually emerging. Up to this time, there are known at least two distinct phases of a 2DEG: the quantum Hall liquid and the Hall insulator. A quantum Hall liquid is characterized by a quantized Hall resistance and a vanishing longitudinal resistance. The Hall insulator, on the other hand, has a diverging longitudinal resistance and a finite Hall resistance. However, the properties of high mobility 2DEG at filling factor 1/2 does not fit into the description of either. Thus behind the wonderful body of physics we learned and developed since 1981, there remains a fundamental unsolved issue, namely, the physics at half-filling.

The efforts during the past year were spent on two problems. The first of these deals with the behavior of a 2DEG at filling factor 1/2. When a 2DEG (i.e. a layer of electrons trapped between the interface of two semiconductors) is submitted to a strong magnetic field of a particular value, it behaves as if there were no magnetic field. How is this to be explained? This difficult problem has remained open for several years. The efforts during the past year resulted in a symmetry argument, that significantly restricted the possible behavior of the system. Using the National High Magnetic Field Laboratory facilities at Los Alamos, H-W Jiang and coworkers at UC Los Angeles have recently observed that the electron and hole resistivity are mirror symmetric about half filling, confirming that the symmetry predicted in this study is indeed there at half filling. Recently there is an increase in the

theoretical efforts on the problem described above, and slowly it is realized that the conventional wisdom is inadequate. The reason that this research is important is because it has potential impact on a 20 years-old consensus, namely that in two space dimensions there is no metallic phase.

The second problem considered during the past year concerned the superconductivity in carbon nanotubes and the metallic stripes in La-Nd-Cu-O high temperature superconductors. A carbon nanotubes is a giant cylindrical molecule formed by carbon atoms. The metallic stripe in the oxide superconductor is a river of electrons in an insulating background. Both of these systems are one-dimensional. We find that due to the one-dimensionality and the strong repulsion between electrons, superconductivity is greatly enhanced in these systems. This research not only reveals the physics of electronic correlation in two very relevant physical systems, but also can have potential impact on the nanoscale application of these materials.

## Refereed Publications

1. Z. Wang, B. Jovanovich, and D-H Lee, "Critical Conductance and Its Fluctuations at Integer Hall Plateau Transitions," *Phys. Rev. Lett.*, 77, 4426 (1996).
2. Y-C. Kao and D-H. Lee, "Bulk Versus Edge in Quantum Hall Effect," *Phys. Rev.*, B 54, 16903 (1996).
3. D-H. Lee, Y. Krotov, J. Gan, and S.A. Kivelson, "Composite Fermion Hall Conductance at  $\nu=1/2$ ," *Phys. Rev.*, B 55, 15552 (1997).
4. Y. Krotov, D-H. Lee, and S.G. Louie, "Low Energy Properties of the (n,n) Carbon Nanotubes," *Phys. Rev. Lett.*, 78, 4245 (1997).
5. Y. Krotov, D-H. Lee, and A. Balatsky, "Superconductivity in Metallic Stripes," *Phys. Rev.* B (accepted).

6. D-H. Lee, "Neutral Fermions at Half-Filling," *Phys. Rev. Lett.* (submitted).

## Presentations

1. D-H. Lee, "Metallic Phases in Quantum Hall Regime," Conference on Low Dimensional Field Theory, Institute of Theoretical Physics, Santa Barbara, CA, 1997 (invited).

## **9744(5) Research and Education Utilizing the NHMFL: Calorimetric Study of Flux-Lattice Melting in YBCO**

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## Abstract

A magnetic field,  $H$ , penetrates a superconductor in magnetic vortices. In this vortex state, each vortex carries a single quantum of magnetic flux, and the density of vortices varies with  $H$ . The vortices are acted on by a Lorentz force in the presence of a finite electric current, causing them to move and dissipate energy, i.e. produce a finite resistance, if the Lorentz force exceeds some critical value. In conventional superconductors the vortices are locked into a rigid lattice that persists to the transition to the normal state at a well-defined critical field  $H_{c2}(T)$ , even in the

presence of substantial electric currents. In the high- $T_c$  cuprate superconductors there is a low- $T$  region in the  $H$ - $T$  phase diagram in which the vortices are fixed, but there is also a high- $T$  region that extends from  $H(T)$  to a lower phase boundary at  $H_m(T)$ . In that part of the phase diagram the vortices are mobile and for finite currents the electrical resistance is not zero. The transition between these two regions has attracted considerable attention both because of the implications for practical superconducting devices and also for the interest in the basic physics of a novel, and in some respects unique, phase transition. Theoretical work suggests that in sufficiently perfect samples the transition would be a thermodynamic first-order transition analogous to the solid/liquid melting transition, in which case it should be accompanied by a latent heat,  $L$ . Observation of a latent heat has been widely recognized as definitive proof of the occurrence of a thermodynamic first-order transition. Preliminary measurements of the latent heat in low magnetic fields have been made at UC Berkeley. The next step in this program is to extend the measurements to a higher magnetic field region using the 20T National High Magnetic Field Laboratory (NHMFL) magnet in which additional important features of the phase diagram can be expected to be found. Detailed plans for the necessary instrumentation at the NHMFL in Los Alamos, and for the participation of the LANL personnel in the project were made in July. The design for inserting the crystal into the 20T magnet was developed shortly thereafter, and the insert is currently being fabricated at UC Berkeley. The insert will be tested for vacuum tightness, functioning of the electrical leads and sample holder, etc., at UC Berkeley. The expectation is to have it ready for initial experiments at LANL in late December of 1997, or January 1998, depending on scheduling of the 20T magnet.

## **9744(6) Research and Education Utilizing the NHMFL: High Field Studies of Strong Correlated Electron Systems**

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*Graduate Students: Robert P. Dickey and Eric Bauer (UC San Diego).*

### **Abstract**

One of the main objectives of our research has been the study of superconductivity and magnetism, and the striking effects that arise from the interplay between these two phenomena. Our research consists of the synthesis and study of novel f-electron systems and high  $T_c$  cuprate superconductors. It involves performing electrical resistivity and magnetization measurements on these materials in high magnetic fields and at low temperatures using the National High Magnetic Field Laboratory (NHMFL) facilities of the Los Alamos National Laboratory. Part of our research has concentrated on the anomalous physical properties of certain rare earth and actinide compounds in which the localized f-electron and conduction electron wavefunctions are strongly hybridized. A remarkable subclass of these compounds consists of metals in which the conduction electrons have enormous effective masses as large as several hundred times the mass of the free electron. Heavy electron materials have attracted worldwide attention, because some of them display an unusual type of superconductivity that may be the analogue of the "triplet" superfluidity found in liquid  $^3\text{He}$  at very low temperatures. Another emphasis of

our research is on copper oxide superconductors, some of which exhibit superconductivity at temperatures as high as  $\sim 130$  K, well above the boiling point of liquid nitrogen (at 77 K). These remarkable superconducting materials are of immense interest because of their potential applications in technology, and the possibility that a new superconducting electron pairing mechanism, different than the conventional electron-phononinteraction, is responsible for their spectacularly high superconducting transition temperatures.

During the past year, we designed and fabricated a new sample holder for electrical resistivity measurements to be used with the 20 tesla superconducting magnet at the NHMFL in Los Alamos. The system was tested by performing an experiment at low temperatures. We found that the sample holder worked extremely well at temperatures as low as 20 mK, and in fields up to 18 T. The thermal contact between the samples and the thermometer was evidently very good. Once the sample holder was operational, we were able to carry out a few experiments on two systems of strongly correlated f-electron materials, the non-Fermi liquid systems  $\text{U}_{1-x}\text{M}_x\text{Pd}_2\text{Al}_3$  ( $\text{M} = \text{Y}, \text{Th}$ ).

### **Refereed Publication**

1. E.J. Freeman, M.C. de Andrade, R.P. Dickey, and M.B. Maple, "Non-Fermi Liquid Behavior in the  $\text{U}_{1-x}\text{Y}_x\text{Pd}_2\text{Al}_3$  System," *Physical Review B* (in preparation).

### **Presentations**

1. R.P. Dickey, M.C. de Andrade, E.J. Freeman, F.G. Aliev, A.H. Lacerda, and M.B. Maple, "Low Temperature Magnetoresistance in the Non-Fermi-Liquid Alloys  $\text{U}_{0.9}\text{Th}_{0.1}\text{Be}_{13}$ ,  $\text{U}_{1-x}\text{Th}_x\text{Pd}_2\text{Al}_3$ , and  $\text{U}_{1-x}\text{Y}_x\text{Pd}_2\text{Al}_3$ ," American Physical Society meeting, Los Angeles, CA, March 15-20, 1998 (contributed).

2. E.J. Freeman, M.C. de Andrade, R.P. Dickey, and M.B. Maple, "Observation of Non-Fermi Liquid Behavior in the  $U_{1-x}Y_xPd_2Al_3$ ," American Physical Society meeting, Los Angeles, CA, March 15-20, 1998 (contributed).
3. R.P. Dickey, E.J. Freeman, M.C. de Andrade, N.R. Dilley, M.B. Maple, and A.H. Lacerda, "Non-Fermi-Liquid Properties of  $U_{1-x}M_xPd_2Al_3$  ( $M = Th, Y$ )," The International Conference on Strongly Correlated Electron Systems, Paris, France, July 15-18, 1998 (contributed).

### **9744(7) Research and Education Utilizing the NFMFL: Thin Films of $C_{60}$**

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#### **Abstract**

A decade after the discovery of fullerenes, questions remain regarding the fundamental properties of  $C_{60}$ , the most prominent fullerene. One of the questions concerns the electronic structure of  $C_{60}$  under extreme conditions such as high pressure and high magnetic fields. Prompted by reports from the Soviet Union regarding unexpected be-

havior of  $C_{60}$  in high magnetic fields, we initiated a joint project whose objective was to investigate changes in absorption spectra, nonlinear optical properties, and photoconductivity of  $C_{60}$  in high magnetic fields. The efforts in this fiscal year were focused on detecting changes in absorption spectra of a thin film of  $C_{60}$  in ultra-high magnetic fields generated by the DIRAC II series at the National High Magnetic Field Laboratory (NFMFL) at Los Alamos. DIRAC II was the second set of very unique explosive flux compression experiments that Los Alamos carried out jointly with Russian scientists. These highly specialized, world-record experiments have been occurring annually at Los Alamos with NFMFL co-sponsorship in which behavior of matter under extremely high magnetic fields is studied. The UC-DRD program arranged for us to participate in these. In experiments lasting a few microseconds, magnetic fields of up to 800 T were achieved. In preparation for the  $C_{60}$  experiment, we developed a method for epitaxial growth of  $C_{60}$  thin films on the tip of an optical fiber. We also designed and optimized an optical set-up, fast and sensitive enough to record transient absorption spectra of  $C_{60}$  during several microseconds of a DIRAC "shot." After successful preparations, which included practice shots on the 50 Tesla magnet at Los Alamos, there were two successful DIRAC experiments involving thin films of  $C_{60}$  and a portion of the  $C_{60}$  spectrum in the high magnetic field has been recorded. A large bulk of numerical data is being processed at this point and will be correlated with the magnetic susceptibility measurements on  $C_{60}$  obtained under the same experimental conditions.

#### **Refereed Publications**

1. A.P. Saab, V. I. Srdanov, B. Marshall, W. Lewis, L. Campbell, J.D. Goettée, D.G. Rickel, and Y. Kim, "Absorption Spectra of  $C_{60}$  in High Magnetic Fields," *Synthetic Metals* (in preparation).

## Presentation

1. A.P. Saab, V.I. Srdanov, B. Marshall, W. Lewis, L.Campbell, J.D. Goettee, D.G. Rickel, and Y. Kim, "Absorption Spectra of  $C_{60}$  in High Magnetic Fields," International Conference on Synthetic Metals (ICSM 98), Montpellier, France, July 12-18, 1998 (contributed).

the high-field phase, and to characterize it for the spin-Peierls material  $(TMTTF)_2PF_6$ . Evidence for a spin gap does not appear until temperatures below about 17K, indicating the onset of a spin-Peierls phase. Nuclear spin lattice relaxation rate data to 18T were collected at the NHMFL Pulsed Field Facility in Los Alamos, and spectral information to 22T was collected at the FSU NHMFL facility. The samples were  $^{13}C$ -labelled on the bridging carbons of the dimer molecule.

## 9744(8) Research and Education Utilizing the NHMFL: High-Field NMR Measurements of the Spin-Peierls Phase of $(TMTTF)_2PF_6$

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From these experiments, we were able to identify the onset field and structure of the high-field phase, to map out a field-temperature phase diagram, and to characterize the relaxation processes in high magnetic fields. We have indications in recent UC Los Angeles experiments at low-fields that high-pressure can be used to reduce the magnetic field for onset by as much as 60%, which will make most of the high-field work accessible to us at the Los Alamos facilities. Our focus for the remainder of our project will be for experiments using fields between 9-18T and at high pressure.

We are the only users at the 20T LANL facility to apply NMR techniques. The magnet is quite adequate for many applications in solid state physics NMR. Our own work is driven by the interest in quantum magnetism. The organic compounds we are examining have some unique features which are proving to be very valuable, including the tunability of properties using pressure and magnetic field. Our long term goal is to demonstrate not only the feasibility of the facility for NMR but to participate in helping to make it more accessible to other users.

## Abstract

The spin-Peierls transition occurs in a few quasi-one dimensional antiferromagnetic (AF) systems in which local spin singlets form with a relatively small gap between the ground state and magnetic excited states. In principle, high magnetic fields can create these magnetic excitations. Our  $^{13}C$  nuclear magnetic resonance (NMR) experiments at the National High Magnetic Field (NHMFL) facilities at the Florida State University (FSU) and Los Alamos National Laboratory were conducted to find evidence for

## Refereed Publication

1. S.E. Brown, W.G. Clark, B.J. Klemme, F. Zamborszky, G. Kriza, C. Merlic, P. Kuhns, and W.G. Moulton, " $^{13}C$  NMR Study of the High-Magnetic Field/Low Temperature Phase of  $(TMTTF)_2PF_6$ ," *Phys. Rev. Lett.* (accepted).

## Presentations

1. S.E. Brown, "Spin-Peirls Phase and Fluctuation Effects in  $(TMTTF)_2PF_6$ ," American Physical Society Meeting, Los Angeles, CA, March, 1998 (invited).
2. S.E. Brown, "Spin-Peirls Phase of  $(TMTTF)_2PF_6$  in High Magnetic Fields," New Energy and Industrial Technology Development Organization (NEDO) Workshop, Los Angles, CA, March, 1998 (invited).
3. S.E. Brown, "Spin-Peirls State and Anti-ferromagnetism in  $(TMTTF)_2PF_6$ ," Workshop on One-Dimensional Magnets and Conductors, UCLA, Los Angeles, CA, March, 1998 (invited).
4. S.E. Brown, "Incommensurate Spin Structures in  $(TMTTF)_2PF_6$ ," Stripes '98, University of Rome, Rome, Italy, June, 1998 (invited).

## **9744(9) Research and Education Utilizing the NHMFL: Measurements at High Magnetic Fields on Correlated-Electron Materials**

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## Abstract

The way electrons move and interact in materials is of fundamental importance and has tremendous implications on future devices which depend on electronic transport. In some exotic systems, correlations between the electrons are strong and lead to a metallic paramagnetic ground state with enhanced thermodynamic parameters at low temperatures. Usually the properties of a ground state resulting from electron-electron interactions are described by a well established theory, which is referred to as Fermi-liquid theory; however, recently approximately a dozen systems have been identified that display non-Fermi liquid behavior. In almost all of these systems the electron's spin is involved in the interaction, and since a magnetic field couples to the spin, measuring the system's properties in an applied field can provide useful information about the strong electron correlations.

A calorimeter and insert were built for the superconducting magnet at the National High Magnetic Field Laboratory in Los Alamos. With this apparatus, the field-dependent specific heat was measured from 1.5 K to 20 K on small single crystals of  $LuNi_2B_2C$  and  $YbNi_2B_2C$  in fields up to 18 T. These compounds are both members of an intermetallic borocarbide series where an interesting interplay between superconductivity and local-moment magnetism occurs. In  $LuNi_2B_2C$  the magnetism is completely suppressed leaving a superconducting ground state with a transition temperature of 16 K, while  $YbNi_2B_2C$  is unique in that it is the only member of the series with an enhanced Fermi-liquid ground state and no long-range order. Magnetic vortices are formed in the superconducting state of  $LuNi_2B_2C$  when the applied field exceeds a critical value. At the center of each vortex is a nonsuperconducting core, and the properties of the core depend on the nature of the superconducting state. Thermal excitations of the normal electrons in the core can be observed in the low-temperature specific heat. Our measurements of the field depen-

dent Sommerfeld coefficient, which is a gauge of the normal component, imply the superconducting gap is anisotropic with line nodes. At low temperatures, there is a feature in the specific heat of  $\text{YbNi}_2\text{B}_2\text{C}$  that is associated with its enhanced Fermi-liquid ground state. In a sufficiently strong applied field, this feature was modified in a way that is qualitatively consistent with the thermal excitations of an uncorrelated-electron gas in the presence of a magnetic field. A quantitative analysis of this observation with a comparison to previously obtained transport data is underway. Finally, magnetotransport measurements were performed on  $\text{UCu}_{5-x}\text{Pd}_x$  with  $x = 1$  and 1.5, where the thermodynamic and transport properties are not describable as a Fermi liquid. At low fields the resistance has a quadratic field dependence. This is predicted by some theories for non-Fermi liquid behavior; however, the prefactor seems to be anomalously small implying the energy scale that characterizes the magnetotransport is much larger than the one for the thermodynamic properties.

### Refereed Publications

1. W.P. Beyermann, A.H. Lacerda, and P.C. Canfield, "Field-Dependent Response of the Heavy Fermi-Liquid Ground State in  $\text{YbNi}_2\text{B}_2\text{C}$ ," *Phys Rev B* (in preparation).
2. G.M. Schmiedeshoff, J.A. Detwiler, W.P. Beyermann, A.H. Lacerda, P.C. Canfield, J.L. Smith, "Critical Fields and Superconducting Properties of  $\text{LuNi}_2\text{B}_2\text{C}$ ," *Phys Rev B* (in preparation).

### Presentations

1. W.P. Beyermann, A.H. Lacerda, and P.C. Canfield, "Field-Dependent Response of the Heavy Fermi-Liquid Ground State in  $\text{YbNi}_2\text{B}_2\text{C}$ ," The International Conference on Strongly Correlated Electron Systems, Paris, France, July 15-18, 1998 (contributed).

2. W.P. Beyermann, A.H. Lacerda, and P.C. Canfield, "Field-Dependent Response on the Heavy Fermi-Liquid Ground State in  $\text{YbNi}_2\text{B}_2\text{C}$ ," The International Conference on Strongly Correlated Electron Systems 1998, Paris, France, July 15 - 18, 1998 (contributed).

3. W.P. Beyermann, A.H. Lacerda, and P.C. Canfield, "Specific Heat and Transport in  $\text{YbNi}_2\text{B}_2\text{C}$  at High Magnetic Fields," The VI Prague Colloquium on f-Electron Systems, Prague, The Czech Republic, July 11 - 14, 1998 (invited).

## **9745 Integrating Los Alamos National Laboratory's Transportation Analysis Simulation System (TRANSIMS) and UC Riverside's Comprehensive Modal Emissions Model**

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## Abstract

It has become apparent in the past few years that significant improvements are needed in our ability to characterize emissions from vehicles traveling on our roadways. Numerous studies have shown that under most on-road operating conditions actual vehicle emissions can differ dramatically from what is predicted by current transportation and mobile source emission models. The primary problem lies in the fact that both transportation models and emission models used to date lack the level-of-detail required to produce accurate emissions inventories. As a result, the following two major programs have been initiated to develop both a better transportation simulation model and a better set of emission models: 1) LANL researchers are currently developing a high level-of-detail traffic simulation model that can be applied to large regional networks. This research is sponsored by the Federal Highway Administration (FHWA) and is known as the Transportation Analysis Simulation System (TRANSIMS) project. When complete, the TRANSIMS model will be used for traffic flow analysis, traffic planning, transportation control measure evaluation, and air quality impacts. 2) Researchers at UC Riverside, College of Engineering-Center for Environmental Research and Technology are currently developing a comprehensive modal emissions (CME) model that predicts emissions output as a function of vehicle operating mode (e.g., idle, cruise, various levels of acceleration and deceleration, etc.). In this program, highly time-resolved emissions and vehicle operation data are being collected through state-of-the-art dynamometer testing for a wide range of vehicle technology types (300+ vehicles). These data are then being used to establish and calibrate a set of analytical functions that describe the physical phenomena associated with vehicle operation and emissions production. The primary objective of this UCDRD project is to integrate LANL's TRANSIMS and UC Riverside's CME models in order to establish a powerful tool that can produce accurate emission inventories. In the first year of research, both teams have generated a detailed

list of interfacing issues and have created a preliminary methodology for integrating the two models. This methodology will be refined in subsequent years of research. Once the two models have been successfully integrated, it will be possible to use the models together to produce accurate emission inventories for both "microscale" (e.g., intersections, highway links) and "macroscale" (i.e., regional level) traffic scenarios. The resulting modeling tool will be very important particularly in light of the conformity requirements of the Clean Air Act Amendments of 1990 and the aggressive implementation of transportation control measures, intelligent transportation systems, alternative fuel vehicles, and more sophisticated inspection/maintenance programs contained in most state air quality management plans.

## Refereed Publication

1. M. Barth, "Integrating a Modal Emissions Model into Various Transportation Modeling Frameworks," *Proceedings of the American Society of Civil Engineers' Transportation and Air Quality III Conference*, Lake Tahoe, CA, August 1997.

## Non-Refereed Publication

1. Portions of work to appear in Transportation Research Board, National Cooperative Highway Research Program Project 25-11 Final Report, August, 1998 (in preparation).

## Presentation

1. M. Barth, "Integrating a Modal Emissions Model into Various Transportation Modeling Frameworks," American Society of Civil Engineers' Transportation and Air Quality III Conference, Lake Tahoe, CA, August 14-17, 1997 (contributed).

## **9746(1) Integrated Catalysis Program: Overview**

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### **Abstract**

A catalyst accelerates the rate of a chemical reaction toward equilibrium. Catalysis

provides economic advantages by allowing chemical reactions to occur more rapidly, thus reducing capital outlay, reducing energy costs, and reducing waste generation. Catalysis cuts across all U. S. industries; products from catalysis account for 20-30 % of the Gross Domestic Product. From a scientific standpoint, catalysis is a rich, multidisciplinary field, combining the elements of chemistry, biochemistry, chemical engineering, theory, and materials science. The studies of catalysts in our program can have an impact on new, environmentally benign, energy efficient chemical processes, and will develop new techniques and tools for the examination of complex materials. These new capabilities will have an impact on the field of catalysis, because the study of heterogeneous catalysts is handicapped by the dearth of useful tools to describe complex materials at the level of detail required. These same tools will probably prove to be valuable for certain aspects of the Department of Energy's Science-Based Stockpile Stewardship program.

The goal of our research in the field of catalysis is to integrate the expertise of the Los Alamos National Laboratory and the UC Campuses to solve difficult problems in the area of synthesis and structural characterization of catalysts using unique experimental facilities and theoretical expertise at Los Alamos and the strengths in materials, chemistry, and catalysis at the university campuses.

This project is focused on three strategies or areas directed at the preparation and/or characterization of microporous molecular sieve materials such as zeolites or phosphates containing catalytically active metal species. One strategy is to prepare and study metal ions isomorphously substituted into microporous frameworks. The second area is the structure and dynamics of small metal clusters isolated in the supercages of zeolites. A third area addresses the synthesis of new and novel microporous frameworks in which the metal component in the microporous framework is potentially catalytically active. At Los Alamos, the work on this project is directed at using experimental techniques, including

screening of catalytic activity, solid-state nuclear magnetic resonance spectroscopy, inelastic neutron spectroscopy, and neutron scattering techniques, to describe the local and long range of the subject metal-containing microporous molecular sieves. The interpretation of some of these results often requires theoretical approaches to model and simulate these complex materials.

Descriptions of individual projects carried out under this program are provided separately in this report by the investigators of these projects. These describe recent results on several classes of catalytic materials. In each of these areas, there is work going on at both the campuses and at Los Alamos. The classes of materials that have been studied are: 1). Titanosilicalites and Ti/Si/O Frameworks, for which we report on neutron scattering studies of TS-1 (LANL), fundamental reaction chemistry of Ti/Si/O frameworks and development of new methods for preparing Ti/Si/O frameworks (UC Irvine), solid state titanium nuclear magnetic resonance and inelastic neutron spectroscopic studies of adsorbates on TS-1 (LANL); 2). The Chemistry of Rh<sub>6</sub>/NaY Catalysts, for which we report on recent progress in experimental and theoretical studies of nuclear magnetic resonance spectroscopy of Xe in microporous materials (LANL and UC Davis) and some preliminary results from novel neutron scattering studies of Rh<sub>6</sub>/NaY (LANL); and 3). Microporous Phosphate Materials as Potential Oxidation Catalysts, for which we report on recent progress on the synthesis of new tin and antimony phosphates (UC Santa Barbara), and describe recent theoretical studies of the nature of cobalt sites in aluminum phosphates and their interaction with molecular oxygen (LANL).

### Refereed Publications

1. S.L. Anderson., J. Szanyi, M.T. Paffett, and A.K. Datye, "Hydrogenolysis and Isomerization of N-Butane on Low-Index Pt Single-Crystals and Polycrystalline Pt Foil," *Journal of Catalysis*, 159, 23 (1996).

2. J. Szanyi and M.T. Paffett, "The Adsorption of Carbon-Monoxide on H-ZSM-5 and Hydrothermally Treated H-ZSM-5," *Microporous Materials*, 7, 201 (1996).
3. J. Szanyi and M.T. Paffett, "The Adsorption of NO And Reaction of NO With O<sub>2</sub> on H-ZSM-5, NaH-ZSM-5, CuH-ZSM-5, and Cu-ZSM-5 : An In-Situ FTIR Investigation," *Journal of Catalysis*, 164, 232 (1996).
4. J. Szanyi and M.T. Paffett, "FT-IR Investigation of the Co-adsorption of Acetonitrile and Carbon-Monoxide on Cu-ZSM-5," *J. Chem. Soc. Faraday Transactions*, 92, 5165 (1996).
5. H. V. Brand, A. Redondo, and P.J. Hay, "Theoretical Studies of CO Adsorption on H-ZSM-5 and Hydrothermally Treated H-ZSM-5," *J. Mol. Catalysis A*, 121, 45 (1997).
6. A. Labouriau and W. L. Earl, "Titanium Solid-State NMR In Anatase, Brookite and Rutile," *Chem. Phys. Lett.*, 270, 278-284 (1997).
7. J. Szanyi and M.T. Paffett, "Co-Adsorption of Acetone and CO on Cu-ZSM-5: An In Situ FTIR Study," *Catalysis Letters*, 43, 37 (1997).
8. W.L. Perry, J.D. Katz, D. Rees, M.T. Paffett, and A.K. Datye, "Kinetics of the Microwave-Heated Carbon Monoxide Oxidation Reaction Over Alumina Supported Pd and Pt Catalysts," *J. Catal.*, 171, 431, (1997).
9. H.V. Brand, A. Redondo, and P.J. Hay, "Theoretical Studies of CO and NO Adsorption on Cu<sup>+</sup>-ZSM-5 Zeolite," *J. Phys. Chem.*, B 101, 7691 (1997).
10. A. Labouriau, T.J. Higley, and W.L. Earl, "Chemical Shift Prediction in the <sup>29</sup>Si MAS NMR of Titanosilicates," *J. Phys. Chem.*, B 102, 2897, (1998).

11. W.L. Earl, B.C. Gates, W. Weber, and A. Laboriau, "Variable Temperature  $^{129}\text{Xe}$  Chemical Shifts: Evidence for Multiple Adsorption Sites in Zeolite Y," *J. Am. Chem. Soc.* (in preparation).
12. W. L. Earl, "Measurements and Calculations of Titanium Electric Field Gradients as a Means of Measuring Solid Structures," *J. Am. Chem. Soc.* (accepted).
8. W.L. Earl, "Probing Zeolite Internal Structures Using Very Low Temperature  $^{129}\text{Xe}$  NMR," International Zeolite Conference, Baltimore, MD, July 5-10, 1998 (contributed).
9. W.L. Earl, "What We Know and Don't Know About Titanosilicalites From Multinuclear NMR Spectroscopy," International Zeolite Conference, Baltimore, MD, July 5-10, 1998 (contributed).

## Presentations

1. M.T. Paffett, "Various Aspects of In-Situ Studies of Zeolites," Catalysis Gordon Research Conference, New London, NH, June 1996 (contributed).
2. W.L. Earl, "Structural Studies of Solids by Ti NMR," 10th Department of Energy/Office of Basic Energy Sciences Conference on Catalysis, Del Lago, TX, May 1996 (contributed).
3. K.C. Ott, "Neutron Scattering and NMR Studies of Titanosilicates," 15th North American Meeting of the Catalysis Society, Chicago, IL, May 1997 (contributed).
4. K.C. Ott, "Neutron Scattering and NMR Studies of Titanosilicates," NATO/Advanced Studies Institute, Villamoura, Portugal, June 1997 (contributed).
5. P.J. Hay, "Theoretical Studies of Selective Oxidation and Hydrocarbon Cracking In Zeolite Catalysts," Zeolite Gordon Research Conference, Plymouth, NH, June 1997 (contributed).
6. P.J. Hay, "A New Embedding Model for Quantum Chemical Simulations of Aluminophosphates." Zeolite Gordon Research Conference, Plymouth, NH, June 1997 (contributed).
7. W.L. Earl, "Nuclear Magnetic Resonance Characterization of Titanosilicate Structures," 15th Meeting of The North American Catalysis Society, Chicago, IL, May 1997 (contributed).
8. W.L. Earl, "Kinetics of Zeolite Dealumination In Steam," International Zeolite Conference, Baltimore, MD, July 5-10, 1998 (contributed).
9. W.L. Earl, "Xenon NMR In Pores: Observations on NMR Chemical Shifts as a Function of Temperature," 37th Rocky Mountain Conference on Analytical Chemistry, Denver, CO, July 1997 (contributed).
10. W.L. Earl, "Use of Titanium And Silicon NMR To Elucidate Structures of Titanosilicates," Dow Chemical Co., Midland, MI, November 1996 (invited).
11. W.L. Earl, " $^{129}\text{Xe}$  NMR and Adsorption to Characterize Zeolite Pores," Michigan Catalysis Club, Detroit, MI, November 1996 (invited).
12. W.L. Earl, "Variable Temperature Xenon NMR from 25 To 300 K in Zeolite Pores," 38th Experimental Nuclear Magnetic Resonance Conference, Asilomar, CA, March 1998 (contributed).
13. M.T. Paffett, "Competitive Adsorption of Molecular Adsorbates on Cu-ZSM-5: A Combined In Situ FTIR Spectroscopic and Theoretical Study," Western States Catalysis Conference, Denver, CO, March 1996 (contributed).
14. M.T. Paffett, "The Adsorption of NO and Reaction of NO With  $\text{O}_2$  on H-, NaH-, CuH-, and Cu-ZSM-5: An In Situ FTIR Investigation," Pacific Basin Conference, Honolulu, HI, December 1996 (contributed).

17. K.C. Ott, "Neutron Scattering and NMR Studies of Titanosilicates," Chemical Engineering Seminar, UC Berkeley, Berkeley, CA, to be scheduled, (invited).
18. P.J. Hay, "Theoretical Studies of Hydrocarbon Cracking In Zeolites," Spring 1997 American Chemical Society Meeting, San Francisco, CA, April 1997 (contributed).
19. P.J. Hay, "Overview of Catalysis Activities at Los Alamos," National Science Foundation-Department of Energy Workshop on Catalysis, San Francisco, CA, April 1997 (invited).
20. A. Redondo, "Embedding Quantum Mechanical Cluster Calculations in a Classical Forcefield," Workshop on Interatomic Potentials and Linking Scales, Institute For Theoretical Physics, UC Santa Barbara, May 1997 (invited).
21. M.T. Paffett, "Various Aspects of In-Situ Studies of Zeolites," Western States Catalysis Conference, Denver, CO, June 1997 (contributed).
22. K.C. Ott, "Neutron Scattering and NMR Studies of Titanosilicates," Florida Catalysis Meeting, Palm Coast, FL, April 1998 (invited)

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## Abstract

The collaboration between the UC Irvine group and Los Alamos has focused on TS-1, a microporous titanium silicalite having 2-3 atomic percent Ti isomorphously substituted onto the tetrahedral Si sites that make up the zeolite framework, and soluble molecular analogs of TS-1. TS-1 catalyzes the oxidation of substrates using hydrogen peroxide as the oxidant under remarkably mild conditions. Because of this, much interest around the world has been focused on understanding the chemistry and catalysis of TS-1 and its soluble analogs. Because TS-1 has such a low concentration of Ti in the framework, it is very difficult to gain the desired information at the level of detail necessary to gain some reasonable understanding of its structure and how this structure influences the remarkable chemistry that TS-1 exhibits.

Study of soluble analogs of TS-1 and the chemistry and synthesis of Ti/Si/O frameworks allows additional insight into the structure and function of this class of catalysts and potential new routes into the incorporation of Ti into silicate frameworks.

At Los Alamos, work has focused on developing and using neutron scattering techniques to examine the local and long-range structure of Ti in the framework of TS-1. Using Rietveld techniques for the refinement of structural parameters from powder neutron diffraction data, we have for the first time been able to determine the pattern of site substitution of Ti among the 12 possible sites that Ti may occupy in the complicated structure of the host silicate. Our study indicates that the Ti is located in just 4-5 specific sites out of the possible 12 sites available. This siting has not been born out by theoretical prediction of the Ti siting. These theoretical predictions are based upon thermodynamic considerations, and our results may

## **9746(2) Integrated Catalysis Program: Synthesis and Reactions of Titanosilicates and Ti/Si/O Frameworks**

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indicate that the Ti siting preference is dominated by kinetics effects during the synthesis of the material. We have also focused on the structure of the related Fe compound, and found similar results. Using Inelastic Neutron Spectroscopy, we have obtained data on peroxide and olefin bound to TS-1 and are presently analyzing the data in order to shed light on the local structural features of the active catalyst. If our analyses prove successful, this would be a rare example of the determination of structural features of an active catalyst. In a complementary approach, we have attempted to use solid state nuclear magnetic resonance to define the local structure of Ti in the resting state of the catalyst. The Ti nuclear magnetic resonance (NMR) experiments are very difficult due to the low sensitivity of  $^{47,49}\text{Ti}$  NMR, and so we began by examining materials having a relatively high concentration of Ti and have been stepping down in concentration as our understanding of Ti NMR probe design and experimental conditions has improved. We have examined the three polymorphs of  $\text{TiO}_2$ , and have then moved to compounds having progressively lower Ti contents such as ETS-10 and other titanium silicate minerals. We have made the interesting observation that the Ti NMR spectra do not reflect the local symmetry of the titanium site because these compounds are covalent, not purely ionic. Theory must be called upon to interpret these data. These calculations are in progress. Preliminary results indicate that theory can be used to calculate NMR parameters for these systems, and that it appears promising that we will be able to use theory and NMR to describe the environment at Ti centers, something that would be impossible without the combined experimental-theoretical approach.

Work at UC Irvine has been focused on synthesizing soluble molecular analogs of TS-1 where Ti ions are site isolated within a soluble silicate framework. This work is directed at gaining an understanding of TS-1 via more readily studied solution techniques. Another goal is to understand the chemistry of silicate frameworks and the introduction

of other elements such as Ti into them. While these studies are in their preliminary stages, potential leads are being developed, and some are being sent to Los Alamos for incorporation into porous hosts and catalytic testing. Our goal is to develop a better understanding of the soluble Ti/Si/O framework compounds, and then to incorporate them into solid state structures where the chemistry remains well-defined, but with the interesting properties associated with the solid state analogs.

### **9746(3) Integrated Catalysis Program: Investigation of the Chemistry of $\text{Rh}_6/\text{NaY}$ Catalysts**

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## Abstract

The goal of this project is to gain a better understanding of the structural details of catalysts that consist of small metal clusters entrapped within molecular sieves. Previous work by the UC Davis group has defined syntheses of these catalytic materials, their catalytic activity for hydrocarbon conversions, as well as the structural aspects of the clusters themselves. Elucidation of the interaction of the small metal clusters with their microporous hosts has eluded all attempts at characterization using Extended X-ray Absorption Fine Structure studies and other techniques. This state of affairs is typical for many interesting catalysts, as there are few if any techniques that are reliable for the accurate determination of detailed structure where the active species is very dilute, and by its very nature, disordered within the host material. Recent developments in nuclear magnetic resonance (NMR) and neutron scattering may allow some of the structural details to be investigated, and that is the goal of this project.

In previous work the UC Davis group has shown that well-defined  $\text{Rh}_6$  clusters may be prepared within the confines of a microporous zeolite host and has investigated the catalytic conversions of these model catalysts. There are still many fundamental unanswered questions regarding the interaction of the  $\text{Rh}_6$  clusters with the zeolite host, such as, "what is the orientation of the cluster with respect to the surface, and where are the clusters located within the microporous framework?"

In an attempt to answer the questions regarding the detailed local structure of the rhodium clusters and their interaction with the zeolite host, we have collected neutron scattering data at LANL and at the Rutherford Appleton Laboratory in the UK, and Xe NMR spectroscopy data at LANL on samples that have been carefully prepared and characterized at UC Davis. The Xe NMR data are the first to be obtained for such samples at extremely low temperatures and are beginning to give information about the

interactions between the metal clusters and the zeolite surface. We have also collected low temperature neutron scattering data, but the data analysis is not yet completed.

Using Rietveld analysis of the neutron scattering data obtained at room temperature on  $\text{Rh}_6/\text{NaY}$ , we have located the  $\text{Na}^+$  ions within the micropores. To date, we have been unable to locate any hints of  $\text{Rh}_6$  within the pores. This is probably an indicator that the metal clusters occupy a large number of the possible sites, and also that there may be a large number of orientations of the cluster with respect to the surface. Alternately, the clusters may be mobile within the cages at room temperature, thus "smearing" out the site populations among a large number of sites and orientations. We are attempting to extract the diffuse scattering information from this data that is related to the disorder of the system. We are currently examining the data for perturbations of the Na siting by the  $\text{Rh}_6$  clusters that might reveal  $\text{Rh}_6$  siting. We have just collected neutron scattering data at low temperatures, and have not yet completed the data analysis. Because Rh is of relatively high atomic number, it may be that X-ray diffraction may give us complementary information, and we will be acquiring low temperature x-ray diffraction data on these samples in the near future.

Xe NMR may also be used as a structural probe for the metal clusters in the pores due to adsorption of Xe on the metal clusters at low temperatures. We began this study by characterizing the Xe NMR in  $\text{NaY}$  without the  $\text{Rh}_6$  clusters. These baseline studies of the Xe NMR, carried out from 40 to 350 K have produced some very interesting and unexpected results that are to be published. Because we have studied the system over a much wider temperature range than what has been done before, this new information has added to our knowledge of these systems and has altered our thinking about the nature of Xe in porous systems. Thus our conclusions are somewhat different than what appears in the current literature. Observation of Xe NMR over a wide temperature

range has allowed us to better understand and predict the chemical shift of xenon which is a sensitive function of the local environment that the Xe atoms can sample. With these baseline results we will proceed to studying the more complex systems containing the metal clusters using xenon as a probe of local structure.

## Refereed Publications

1. T.-K. Cheung, P.J. Hay, B.C. Gates, and A. Redondo, "Dehydrogenation and Cracking of Ethane in the Presence of USY and of HZSM-5 Zeolites: A Semi-empirical Approach," *Journal of Catalysis* (in preparation).
2. A. Labouriau, T. Pietrass, S. Neugebauer Crawford, W.A. Weber, G. Panjabi, B.C. Gates, and W.L. Earl, "Probing Zeolite Internal Structures Using Very Low Temperature  $^{129}\text{Xe}$  NMR," *Journal of Physical Chemistry B* (in preparation).
3. A. Labouriau, S. Neugebauer Crawford, G. Panjabi, B. Enderle, B.C. Gates, and W.L. Earl, "Probing Rhodium Clusters in Zeolite NaY with Low-Temperature  $^{129}\text{Xe}$  NMR Spectroscopy." *Journal of the American Chemical Society* (in preparation).

## Presentation

1. A. Labouriau, T. Pietrass, S. Neugebauer Crawford, W.A. Weber, G. Panjabi, B.C. Gates, and W.L. Earl, "Probing Zeolite Internal Structures Using Very Low Temperature  $^{129}\text{Xe}$  NMR," International Zeolite Congress, Baltimore, MD, July, 1998 (contributed).

## 9746(4) Integrated Catalysis Program: Microporous Phosphate Materials as Potential Oxidation Catalysts

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## Abstract

The objective of this activity is different than the other activities that are a part of the UC-LANL Integrated Catalysis Project. In the other activities, we strive to describe and understand unique structural features of relatively well-known, but poorly understood systems. This project is directed at discovering new catalytic materials for oxidation catalysis, and also to bring to bear the predictive power of theory to assist in the search for new materials. The objective of the UC Santa Barbara activity is to discover new classes of materials that may catalyze the partial oxidation of hydrocarbons. The Los Alamos effort has been in the elucidation of reaction mechanisms using theoretical techniques. Knowledge of reaction mechanism allows for the improvement of existing catalysts and the design of new materials.

The focus of the UC Santa Barbara group has been in the synthesis of new tin and antimony phosphates and phosphonates. Tin and antimony are known to be important in a number of partial oxidation reactions. Our first successes were in the area of tin

phosphates and phosphonates, where we were able to make the first examples of such materials with open crystalline architectures in which there are channels and cavities, as in the aluminosilicates. During the last 12 months, however, we have concentrated our effort on new phosphates of antimony 3+, which we consider to be more promising candidates as oxidation catalysts. Prior to our work in this area, there were no known antimony 3+ phosphates with open frameworks. Antimony 5+ phosphates with layered structures, however, are well known from the work of Piffard in Nantes and have interesting properties as acidic catalysts (that is to say, for reactions that involve transformations of organic molecules without any oxidation).

We have enjoyed a considerable amount of success during the last 12 months in the search for new phosphates of antimony 3+. Our strategy has been to react antimony 3+ oxide,  $Sb_2O_3$ , with phosphoric acid in the presence of organic amines. Reactions were carried out under hydrothermal conditions (i.e. in superheated water) in the presence of hydrofluoric acid to assist with the dissolution of the antimony oxide. It is intended that the amines should be trapped within the antimony phosphate framework, thus forcing it to adopt an open architecture. Afterwards, it should prove possible to remove the amine, leaving behind a structure that has channels and cavities in which catalytic reactions can take place.

We have synthesized 5 new antimony 3+ phosphate compounds under hydrothermal conditions at pH 5 - 7 and temperatures of 130-160 C. Crystal structures have been determined by single crystal X-ray diffraction. Technical details have been or will be published.

At Los Alamos, our interest in phosphate-based catalysts has been directed at understanding the interaction of dioxygen with metal ions incorporated into the phosphate framework. Computational approaches to catalytic reaction pathways require high quality electronic structure methods.

However, due to their relatively high computational expense, system sizes are often limited to less than fifty atoms. Relatively long-range interactions are often thought to play an important role in stabilizing transition states and reaction intermediates in zeolites which are difficult to consider with traditional quantum chemical methods. Embedding methods, in which short-range interactions are represented quantum mechanically and longer range interactions are handled using molecular mechanics can provide a solution to this difficulty. We have developed a new methodology for embedding in transition-metal substituted systems based on effective core potentials. The advantage of this approach is that one can embed the quantum mechanical cluster system into an ionic description of the background lattice, whereas other approaches require a "splicing" of the bonds in the cluster onto the classical bonds in the lattice. Initial studies have focused on reproducing structural parameters of prototypical aluminophosphate (AlPO) systems. AlPOs are structurally similar to the silicate zeolites, and are of interest to us as microporous hosts for site-isolated catalysts. Results on berlinitite have appeared promising, and we are now trying the embedding technique on larger AlPO systems and those that contain additional metal ions. We have also used these computational techniques to examine the role of local structure on the ability of a framework metal ion to bind oxygen, a reaction step that is crucial for understanding oxidation catalysis.

## Refereed Publications

1. S. Natarajan, M.P. Attfield, and A.K. Cheetham, "[ $NH_3(CH_2)_2NH_3$ ] $^{2+}$  $_{0.5}[Sn_4P_3O_{12}]$  $^-$ : An Open-Framework Tin(II) Phosphate," *Angew. Chemie*, 36, 978-980 (1997).
2. B. Adair, S. Natarajan, and A.K. Cheetham, "Synthesis and Structural Characterization of a Novel Tin (II) Phosphate," *J. Solid State Chem.* (accepted).

**Invited Presentations by  
A.K. Cheetham**

1. "Nanoporous Materials," Chemical Engineering Department, Notre Dame University, IN, January 28, 1997.
2. "Synthesis of Novel Inorganic Framework Structures Using Organic Bases as Structure-Directing Agents" at Florida Advanced Materials Chemistry Meeting, Palm Beach, FL, March 11, 1997.
3. "Recent Developments in Nanoporous Materials," Air Products, Allentown, PA, March 25, 1997.
4. "In Situ Studies of Sol-Gel Synthesis," American Chemical Society Meeting, San Francisco, CA, April 16, 1997.
5. "Characterization of New Open-Framework Silicate and Phosphate Structures," Shell Catalysis Workshop, Valencia, Spain, May 16, 1997.
6. "Recent Developments in the Chemistry of Nanoporous Phosphates," Gordon Research Conference on Zeolites, Plymouth, NH, June 18, 1997.
7. "Recent Developments in Inorganic Materials," Los Alamos National Laboratory, Los Alamos, NM, July 15, 1997.
8. "Recent Developments in Nanoporous Materials," University of Mulhouse, France, October 8, 1997.
9. "Recent Developments in Nanoporous Materials," University of Nantes, France, October 15, 1997.
10. "Nanoporous Materials," University of Caen, France, October 24, 1997.
11. "The Nature and Scope of Inorganic Materials," Samsung Chemical Co., Taejon, S. Korea, October 29, 1997.
12. "Recent Developments in Nanoporous Materials," University of Versailles, France, October 15, 1997.
13. "Recent Developments in Nanoporous Materials," University of Friburg, Switzerland, November 12, 1997.
14. "Recent Developments in Inorganic Materials," University of Lausanne, Switzerland, November 14, 1997.
15. "Synthesis of Open Framework Phosphate Materials Using Organic Structure-Directing Agents," University of Neuchatel, Switzerland, December 15, 1997.

**9747 Hamiltonian Geophysical Fluid Dynamics**

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**Abstract**

As a UC DRD Visiting Scholar, Darryl D. Holm, Los Alamos Laboratory Fellow, spent five months from January to mid-May 1997 at the Institute of Nonlinear Science (INS) and the Mathematics Department at Santa Cruz. This visit had the following results: (1) It built on recent parallel successes by Holm

and Geoff Vallis, INS Director, in the analytical development of a class of ocean and atmospheric circulation models; (2) It renewed and continued collaborations with Tudor Ratiu on global geometry in the Hamiltonian description of ideal fluid dynamics, in the context of geophysical fluid dynamics models of large-scale ocean and atmospheric circulation; and (3) It allowed Holm to share his experience with the faculty and students at UC Santa Cruz by teaching an advanced graduate-level course in the their Mathematics Department entitled Math284, Topics in Dynamics: Hamiltonian Geophysical Fluid Dynamics.

In the realm of education, the UCDRD Visiting Scholar Program produced a successful advanced graduate course experience for six mathematics graduate students and one astrophysics postdoctoral fellow. The Visiting Scholar participated in many academic activities of the UC Santa Cruz Mathematics Department, including participating on the Doctoral Thesis committees for several of the students who took his course.

The main research results of the program were three long fundamental papers containing new mathematical theorems developing the Euler-Poincaré formulation for application to ideal continuum dynamics. These papers were co-authored by the Visiting Scholar with University of California faculty. One of these papers included as co-author a student (Mark Hoyle) from the Visiting Scholar's course. Another student (Shinar Kourenbaeva) came to Los Alamos as a summer Graduate Research Assistant in 1997 and performed research based on the Visiting Scholar's course. This research will also be part of her Doctoral Thesis. The research performed by the Visiting Scholar with his University of California and California Institute of Technology collaborators is the basis for a significant proposal to US DOE for funding through UC.

## Refereed Publications

1. D.D. Holm, J.E. Marsden, and T.S. Ratiu, "The Euler--Poincaré Equations and Semidirect Products with Applications to Continuum Theories," *Adv. Math* (accepted).
2. H. Cendra, D.D. Holm, M.J.W. Hoyle, and J.E. Marsden, "The Maxwell-Vlasov Equations in Euler--Poincaré form," *J. Math. Phys* (accepted).
3. D.D. Holm, J.E. Marsden, and T.S. Ratiu, "The Euler--Poincaré Equations in Geophysical Fluid Dynamics," *Mathematics of Atmospheres and Oceans, Cambridge University Press* (accepted).
4. D.D. Holm, J.E. Marsden, and T.S. Ratiu, "Euler--Poincaré Models of Ideal Fluids," *Phys. Rev. Lett.* (accepted).

## Presentation

1. D.D. Holm, "Hamilton's Principle Asymptotics and Weak Solutions in Geophysical Fluid Dynamics," American Mathematical Society Meeting, Corvallis, OR, April 17-23, 1997 (invited).

## **9748 Silicon Metabolism in Diatoms**

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Postdoctoral Fellow: Yolanda Del Amo (UC Santa Barbara).

Graduate Student: Rebecca Shipe (UC Santa Barbara).

## Abstract

This project is a collaboration that takes advantage of unique facilities and capabilities at LANL and UC Santa Barbara in which new materials and methods are being developed and applied to the laboratory and field study of marine diatom species and their influence on global climate and geochemical cycles. Diatoms are the main primary producers in most coastal marine systems. It is estimated that they contribute to more than 40% of the total marine primary productivity. These photosynthesizing organisms therefore represent a major sink for atmospheric carbon dioxide. Besides the usual nutrients (carbon, nitrogen, phosphorus, etc.) required by autotrophic phytoplankton, diatoms also have an obligate requirement for silicon during critical parts of their cell cycle. Several models reveal that silicon could be the limiting nutrient for diatom proliferation in certain marine environments thereby significantly influencing the level of primary productivity in those systems. In some instances, when silicon becomes the limiting nutrient in an algal bloom, other much less benign species, especially toxin producing dinoflagellates, can become dominant. A quantitative understanding of the physiology of silicon use by diatoms and the role of silicon nutrient limitation on marine algal blooms is thus of practical environmental importance.

To date there have been several significant products of the collaboration. We have developed methods for production of Si-32 in high specific activity for use as a radiotracer

in diatom nutrient studies. Four patents have been issued and one refereed publication has resulted from this work. We have developed and tested new radioanalytical techniques for quantitative measurement of absolute and kinetic uptake of silicic acid by diatoms in the laboratory and in the field. Two refereed publications are in press describing this research. Both principal investigators are serving on the organizing committee of an international workshop on the application of various tracers to marine biogeochemical cycles that will be held in Brest, France in August of 1999. We have obtained support for continuation of the collaboration through the Department of Energy Office of Biological and Environmental Research and continue to develop proposals to extend radioanalytical techniques to the precise correlation of silicon uptake data to carbon primary production. These methods will provide new data pertinent to models developed for understanding the role of diatoms in determining global climate. This collaboration supports research goals of the Department of Energy and the National Science Foundation in the area of climate and environmental research. The work will have significance both from a basic science perspective and for establishment of national policy relative to the effect of greenhouse gases on global climate.

## Refereed Publications

1. M.A. Brzezinski and D.R. Phillips, "Evaluation of Si-32 as a Tracer for Measuring Silica Production Rates in Marine Waters," *Limnology and Oceanography*, 42(#5), 856-865, (1997).
2. M.A. Brzezinski, D.R. Phillips, F.P. Chavez, R.C. Dugdale, and G.E. Friederich, "Silica Production in the Monterey, California Upwelling System," *Limnology and Oceanography* (accepted).

## **9749 Investigations of the Structures of Microtubule-Based Cellular Motors Using Neutron Scattering**

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### **Abstract**

Adenosine Triphosphate (ATP) is the universal currency of chemical energy in biological systems. It is the fuel for muscle contraction, cell motility, biological pumps and cellular "biomotors" which have diverse functions in biology. The long-term goal of our research is aimed at understanding how the chemical energy stored in ATP is converted into movement by cellular motors that move along microtubule (MT) tracks. In this first stage of our work we are measuring the average separation ( $d$ ) between the two (identical) "motor domains" of the dimeric microtubule-based motors non-claret disjunctional protein (*ncd*) and kinesin when free in solution. As these motor domains contain the ATPase and MT binding sites we can test to see whether there is a direct coupling with ATP hydrolysis to produce the large changes in  $d$  required for movement. We are thus now searching for changes in  $d$  of free motors when nucleotide

and nucleotide analogs, which are believed to represent important kinetic intermediates, are bound. In addition, we are looking for differences in  $d$  (and/or dispersion in  $d$ ) between *ncd* and kinesin which would account for the opposite directionality of their movement on microtubules. Eventually we hope to measure *in situ* values of  $d$  when attached to microtubules with different nucleotides and nucleotide analogs present. We expect that the distance information from free and bound motors will give insight into how the two motor domains coordinate to produce motility.

This project studies an important basic science question about energy transduction in biology. In the long run the knowledge obtained may contribute to a further understanding of cancer and heart disease. In the short run we believe that this project will strengthen structural biology and the use of neutron scattering to investigate structural biology at the Los Alamos National Laboratory. As the Los Alamos Neutron Science Center (LANSCE) is just now becoming useful for biological studies, but has little experience in this area, our project will accelerate the ability of others to do such work at LANSCE by solving related physical and logistical problems. In addition, some of the projected work will require the implementation of a method recently proposed by the campus investigator. A successful implementation of this method, which may require significant experimental development, will allow it to be used for other biological problems and perhaps be adapted to neutron studies in other disciplines.

During the eight months this project was funded in FY 1997, the campus investigator established the methodology of large-scale preparation of *ncd* and kinesin dimers in his laboratory. He has learned the best method of storing and transporting these labile proteins. We have had one X-ray scattering run and one neutron run which has allowed us to obtain preliminary scattering data at different ionic conditions and with different analogs present. We have confirmed that

these proteins are indeed dimers (by MW weight measurements). It was found that  $d$  for *ncd* is little affected by actively hydrolyzing ATP or analog addition. However, preliminary evidence indicates a big difference between *ncd* and kinesin scattering. If confirmed by further studies this would be the first evidence of a large-scale difference between *ncd* and kinesin structures and may account for the difference in the directionality of their movement on microtubules.

## **9751 Integrated Structural Biology of Protein-Nucleic Acid Complexes**

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### **Abstract**

We are investigating DNA binding proteins that play essential roles in DNA repair. DNA damage has many causes both spontaneous and induced by environmental insults. The result is genomic instability which often leads to mutations and cancer if not properly repaired. Although there has been substantial progress in the field of DNA repair using biochemical and genetic approaches, the progress in determining the structural basis of damage recognition and repair has been limited. Understanding the role of DNA repair proteins in the maintenance of genetic stability will ultimately require detailed

models of the structure-function relationships and protein interactions responsible for these processes. Atomic force microscopy (AFM) and three-dimensional cryo-electron microscopic (cryo-EM) reconstruction are the only techniques capable of determining the structure of large multi-protein/nucleic acid complexes. Our studies have focused on the application of these techniques to determine the three-dimensional structure of DNA repair complexes in association with DNA. The atomic force microscope (AFM) is a high resolution instrument with several advantages over more traditional microscopic approaches. With the ability to image unstained and uncoated protein-nucleic acid complexes in air, aqueous buffers or organic solvents, the AFM is uniquely suited for biological studies and provides a means by which macromolecular interactions can be visualized under native conditions. In particular, the AFM is useful for the analysis of DNA-protein interactions, DNA conformational changes, and structural studies of large proteins or multi-protein assemblies.

In the first year of this project we have made technical progress at LANL and at UC Davis which has allowed the reproducible high resolution imaging of a key component of the mammalian DNA double-strand break (DSB) repair apparatus and a DNA recombination/repair protein, respectively. We have confirmed the validity of high resolution AFM observations by comparison with three-dimensional models built from cryo-electron micrographs at UC Los Angeles and we have established technology at Los Alamos which will allow the in-house fabrication of carbon nanotube AFM probes. These accomplishments have resulted in the first glimpse of the three-dimensional structure of a DSB repair protein and will form the basis for extending our collaborative investigations into the structure of this and other DNA repair complexes.

## Presentation

1. E.M. Seitz, J.P. Brockman, S.J. Sandler, A.J. Clark, and S.C. Kowalczykowski, "RadA Protein is an Archaeal RecA Protein Homolog that Catalyzes DNA Strand Exchange," Federation of American Societies for Experimental Biology Conference on Genetic Recombination and Genomic Rearrangements, Snowmass, CO, August 2-7, 1997 (contributed).

(Department of Applied Sciences, UC Davis); JorShan Choi (Energy Program Office, Lawrence Livermore National Laboratory).

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*Graduate Students: Jessica Booher, Luca Gratton, Anne Keller, Andrew Koehler, Jennifer Miller, Adam Stone, and Louise Wells (UC Berkeley).*

*Undergraduate Students: John Mitchell and David Hutchinson (UC Berkeley).*

## Abstract

This project aims to develop a new, integrated and comprehensive understanding of the challenges involved in designing and carrying out long-term management strategies for nuclear materials and other technologies with intrinsic complexity and hazard. In part, this work applies analytic approaches from the social sciences and policy analysis to identify requirements and design criteria for management systems that simultaneously consider technical and social-institutional constraints having to do with organizational dynamics, safety, regulation, and public participation in decision processes. This will enable designers of such technical systems to take into account a larger array of factors, including those they have encountered in the past as extrinsic challenges (such as intrusive regulation or public opposition) but have been unable to incorporate into their own work context in a meaningful and practical way. Thus, rather than having to take a reactive stance in a situation fraught with technical and political uncertainties, scientists and policymakers can anticipate and address social and institutional challenges.

Another aspect of the project focuses specifically on the public and expert discourse about nuclear materials management, explaining conflicting accounts and assessments through their particular logical and interpretational contexts. This "discourse

## **9752 Institutional And Technical Issues Regarding Nuclear Stewardship: Radioactive Waste And Nuclear Materials Management**

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analysis" adopted from the discipline of rhetoric and linguistic analysis helps clarify disagreements and points to agreement where it exists, thus providing a needed basis for various participants in the dialogue on controversial technical issues to hear and understand each other.

Over the past year, project researchers have engaged in work with laboratory scientists in various ways, including intensive on-site observation and analysis, cooperative efforts in systems modeling and project evaluation, as well as many interviews and discussions. In addition to publications on preliminary research results that are technical in nature, this work has resulted in the establishment of fertile working relationships across disciplines to make possible an integrated and practical analytic approach drawing on diverse fields of knowledge. This project has also completed analysis of the potential phenomenon of autocatalytic criticality of fissile material disposed in geologic media.

## Refereed Publications

4. L.J. Gratton, W.E. Kastenberg and P.F. Peterson. "Bounding Energy Production Estimates for Autocatalytic Fissile Material Deposits in Geologic Media," *Proceedings of the Topical Meeting on Criticality Safety Challenges in the Next Decade*, American Nuclear Society, Chelan, Washington, September 7-11, 1997, pp. 130-141.
5. E. Greenspan, J. Vujic, and J. Burch, "Neutronic Analysis of Critical Configurations in Geologic Repositories: Part I - Weapons-Grade Plutonium," *Nuclear Science and Engineering*, 127, (no.3), 262-91, November 1997.
6. E. Greenspan, S. Armel, J. Ahn, and J. Vujic, "Critical Depositions of Uranium in Rock Having Positive Reactivity Feedback," *Proceedings of the American Nuclear Society Topical Meeting on Criticality Safety Challenges in the Next Decade*, Chelan, WA, September 7-11, 1997, pp. 51-58.
7. Y. Karni and E. Greenspan, "The SWAN Code for Optimization of Critical Systems," *Trans. American Nuclear Society*, 76, 242 (1997).
8. Y. Karni and E. Greenspan, "The SWAN Code for Minimum Critical Mass and Maximum keff Determination," *Proceedings of the American Nuclear Society Topical Meeting on Criticality Safety Challenges in the Next Decade*, Chelan, WA, September 7-11, 1997, pp. 181-188.
9. W.E. Kastenberg, L.J. Gratton, E. Greenspan, J. Ahn, P. Chambre, D.R. Olander, P.F. Peterson, and J. Vujic, "Possibility for Autocatalytic Criticality of Fissile Materials in Geologic Repositories," *Proceedings of the International Conf. On Future Nuclear Systems, Global '97*, Yokohama, Japan, October 5-10, 1997, pp. 926-930.
10. W.E. Kastenberg and L.J. Gratton. "On the Hazards of Managing and Disposing of High-Level and Transuranic Nuclear Waste," *Physics Today*, 50, No. 26, 41 (June 1997).

11. W.E. Kastenberg, P. F. Peterson, J. Ahn, B. Bessinger, J. Burch, G. Casher, P. Chambre, N.G.W. Cook, F.M. Doyle, E. Greenspan, B. Hilbert, D.R. Olander, and J. Vujic, "Scenario Assessment of Autocatalytic Criticality in Yucca Mountain Geologic Repository," *Proceedings of the Waste Management '97 Conference*, Session 47, Tucson, AZ, March 2-6, 1997.

12. T.H. Kim, N. Z. Cho, and E. Greenspan, "Fuel-Self-Sufficient Heavy-Water Lattices for Proliferation Resistant Multiple Fuel Recycling," *Trans. American Nuclear Society*, 77, 108 (1997).

13. T.R. La Porte and A. Keller. "Assuring Institutional Constancy: Requisite for Managing Long-Lived Hazard," *Public Administration Review*, 56, 6, 535-544 (November/December 1996).

### Non-Refereed Publications

1. T.R. La Porte, "Institutional Elements for Long Term Stewardship in a Nuclear Age: Views from a Stewardee," *Proc. of the Workshop on Land Use and DOE Sites: The Implications for Long Term Stewardship*, sponsored by the Resources for the Future and Environmental Management, DOE, Washington, D.C., January 16-17, 1997.

2. T.R. La Porte, "Evolving High Reliability Organizations and Institutional Strain in Elements of the U.S. Nuclear Future," *Final report LA-UR 97-3227 (covering 1/2/97-6/30/97)* UCB Contract LANL-C14550017-3Y-LAPORT-06/97, July 1997.

3. T.R. La Porte, Editorial, "Institutional Challenges in LANL's Nuclear Future," *Actinide Research Quarterly of the Nuclear Materials Technology Division*, Fall 1997.

4. W.E. Kastenberg and L.J. Gratton, "On the Hazards of Managing and Disposing of High-Level and Transuranic Nuclear Waste," Center for Nuclear and Toxic Waste Management (CNTWM) Report 97-6.

### Presentations

1. E. Greenspan, J. Ahn, E. Elias, W. E. Kastenberg, N. Z. Cho, and T. H. Kim, "Nuclear Energy Systems Having Low Proliferation Risk," International Specialist Meeting on Future Nuclear Energy Systems and Fuel Cycle Options, Tokyo Institute of Technology, Tokyo, Japan, October 13, 1997 (invited).

2. A. Koehler, "System Modeling and Possible Applications for the Social Sciences," Annual Meeting of the International Council on Systems Engineering (INCOSE), Los Angeles, CA, August 5, 1997 (contributed).

3. A. Koehler and M. O'Hare, "The Design of Socio-technical Systems" Annual meeting of the Association of Public Policy and Management (APPAM), Washington, D.C., November 6-8, 1997 (contributed).

4. T.R. La Porte, "Managing Nuclear Materials: The Unexpected Institutional Challenges of Environmental and Stockpile Stewardship," Environment, Safety & Health Division Seminar Series, LANL, June 20, 1997 (invited).

5. T.R. La Porte, "Elements of Institutional Stewardship in the Face of an Emerging Nuclear Future. LANL and 'Pit' Production: Field Notes in an Institution Approaching Transition," Student Organization Studies Seminar Series, Department of Political Science, UC Berkeley, September 1997 (invited).

6. T.R. La Porte, "Management Without End: It's the 'Pits!'" Fourth National Public Management Research Conference, University of Georgia, October 1997 (invited).

7. J. Ahn, E. Greenspan and P. Chambre, "Possibility of Underground Autocatalytic Criticality by Vitrified HLW in Water Saturated Geologic Repositories," *Waste Management '97 Conference*, Session 47, Tucson, AZ, March 2-6, 1997 (contributed).

8. J. Ahn, E. Greenspan, S. Armel, D. Roberts, and P. Chambre, "Possibility for Underground Autocatalytic Criticality by Actinides in Vitrified HLW," International Conference On Future Nuclear Systems, Global '97, Yokohama, Japan, October 5-10, 1997 (contributed).

9. N.E. Brown, J. Hassberger, E. Greenspan, and E. Elias, "Proliferation Resistant Fission Energy Systems," International Conference On Future Nuclear Systems, Global '97, Yokohama, Japan, October 5-10, 1997 (contributed).

10. L.J. Gratton, W.E. Kastenberg, and P.F. Peterson, "Bounding Energy Production Estimates for Autocatalytic Fissile Material Deposits in Geologic Media," American Nuclear Society Topical Meeting on Criticality Safety Challenges in the Next Decade, Chelan, WA, September 7-11, 1997 (contributed).

11. E. Greenspan, S. Armel, J. Ahn, and J. Vujic, "Critical Depositions of Uranium in Rock Having Positive Reactivity Feedback," American Nuclear Society Topical Meeting on Criticality Safety Challenges in the Next Decade, Chelan, WA, September 7-11, 1997 (contributed).

12. Y. Karni and E. Greenspan, "The SWAN Code for Minimum Critical Mass and Maximum  $k_{eff}$  Determination," American Nuclear Society Topical Meeting on Criticality Safety Challenges in the Next Decade, Chelan, WA, September 7-11, 1997 (contributed).

13. W.E. Kastenberg, L.J. Gratton, E. Greenspan, J. Ahn, P. Chambre, D.R. Olander, P.F. Peterson, and J. Vujic, "Possibility for Autocatalytic Criticality of Fissile Materials in Geologic Repositories," International Conference On Future Nuclear Systems, Global '97, Yokohama, Japan, October 5-10, 1997 (contributed).

14. W.E. Kastenberg, P.F. Peterson, J. Ahn, B. Bessinger, J. Burch, G. Casher, P. Chambre, N.G.W. Cook, F.M. Doyle, E. Greenspan, B. Hilbert, D.R. Olander, and J. Vujic, "Scenario Assessment of Autocatalytic Criticality in Yucca Mountain Geologic Repository," Waste Management '97 Conference, Session 47, Tucson, AZ, March 2-6, 1997 (contributed).

## **9753(1) Frontiers of Materials Science Program: Overview**

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### **Abstract**

The aim of the Frontiers of Materials Science Program is to explore frontier areas of interdisciplinary materials science of common scientific and strategic interest to Los Alamos National Laboratory and the National Science Foundation's Materials

Science Laboratory at UC Santa Barbara. This aim is being implemented through mini-grants, awarded competitively, to support specific projects involving graduate students or postdoctoral fellows with mentors at both institutions, and by providing funds to enable researchers to participate in the "Frontiers in Materials Science Seminar Series," in topical workshops, and in new project exploratory discussions. The interdisciplinary character of materials science at UC Santa Barbara and LANL, and their complementary skills and facilities, assists exploration of exciting new frontiers of materials science with maximal efficiency and flexibility, so that these frontier fields can be rapidly assessed for their technology and growth potential, and competencies can be seeded. The excellent educational outreach initiatives at the UC Santa Barbara Materials Science Laboratory combined with the unique research environment at LANL, provide special opportunities for training young researchers in interdisciplinary materials science.

The projects initiated to date include topics in areas of nonlinear, nonequilibrium, multi-scale processes; inorganic-organic interfaces; biomimetic materials; active thin films; complex fluids; soft condensed matter; magnetoresistive materials; neutron scattering; and molecular sieves. New partnerships between numerous LANL divisions and UC Santa Barbara departments are represented. Workshops have been held at both LANL and UC Santa Barbara.

The "Frontier" seminar series which is held in Los Alamos has been extremely popular with LANL staff and has generated serious discussion, at senior management levels, of a specific joint program to study combining organic and inorganic materials. This is of great importance to rational strategies for understanding, controlling and using complexity in electronic and structural materials, with profound impact on classes of materials lying between traditional disciplines of chemistry, solid state physics, materials science, biological sciences, and geoscience.

Descriptions of individual projects carried out under this program are provided separately in this report by the investigators of these projects.

## **9753(2) Giant Magneto-resistance in Metal Oxides**

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### **Abstract**

Giant magnetoresistance (GMR) materials based on the perovskite manganite oxides have attracted a great deal of excitement recently because of the novelty of the basic physics they exhibit, e.g., subtle couplings of spin, charge and lattice driven metal-insulator and magnetic transitions, accompanied by complex phenomena such as charge (polaron) localization, and valence ordering, and the potential for new technology this has created. We are now building on current GMR single crystal and thin film programs at UC Santa Barbara and LANL to explore new classes of potential GMR materials: ferrite spinels; layered manganite compounds; and pyrochlores. The research takes advantage of complementary capabilities at UC Santa Barbara and LANL in synthesis, characterization and modeling. It also provides unique training for student and postdoctoral associates, and competitively positions UC Santa Barbara and LANL for program development in GMR and other functional electronic materials.

Progress during the five months of support made available during 1997 occurred in the areas of new GMR materials and thin films of layered manganates. Our attempts to

synthesize novel GMR materials based upon iron oxide spinels continued at UC Santa Barbara. At the present time, we have been able to reduce Tc to close to room temperature by replacing iron (II) by zinc, but only at the expense of losing the metallic conductivity and the metal to semiconductor transition that are required for GMR. We have recently demonstrated at UC Santa Barbara that epitaxial thin films of GMR materials based on La, Sr, Mn and O can be grown on single crystal (100) strontium titanate substrates by liquid phase epitaxy methods. We are now attempting to extend this approach to the growth of thin films of the layered manganates based upon  $(La, Sr)_3Mn_2O_7$ . For reference purposes we have prepared bulk samples of the layered material and we are now attempting to prepare the thin films.

### Refereed Publications

1. C.N.R. Rao and A.K. Cheetham, "Charge Ordering in Manganates," *Science*, 276, 911-912 (1997).
2. A.D. Polli, F.F. Lange, M.A. Ahlskog, R. Menon, and A.K. Cheetham, "Processing GMR Thin Films via Chemical Solution Deposition," *Journal of Materials Research* (submitted).
3. C.N.R. Rao and A.K. Cheetham, "Giant Magnetoresistance, Charge Ordering and Related Aspects of Manganates and Other Oxide Systems," *Advanced Materials* (accepted).
4. R. Heffner, L.P. Le, D.E. MacLaughlin, G.M. Luke, K. Kojima, B. Nachumi, Y.J. Uemura, G.J. Nieuwenhuys, S-W. Cheong, "Unusual Relaxational Dynamics in  $La_{1-x}Ca_xMnO_3$ ," *Physica B*, 759, 230-232 (1997).
5. A.R. Bishop, H. Röder, "Theory of Colossal Magnetoresistance," *Current Opinion in Solid State and Materials Science*, 2, 244 (1997).

### **9753(3) Study of Island Growth Mode of Epitaxy and Phase Selection of Perovskite Thin Films by Solution Methods**

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### Abstract

Single crystal ferroelectric thin films are preferred to polycrystalline films for a range of optical and electronic applications either for their anisotropic properties or optical pathways. Especially, devices which use optical transmission require films that do not contain light scattering grain boundaries. Perovskite single-crystal thin films, such as  $Pb(Zr_xTi_{1-x})O_3$  and  $Ba_xSr_{1-x}TiO_3$ , i.e., important ferroelectric compositions, can now be produced by Chemical Solution Deposition and Hydrothermal Epitaxy, two solution methods pioneered at UC Santa Barbara. Relative to conventional epitaxial methods, both methods have the advantage of low cost and precise compositional control; one can form single crystal thin films at very low temperatures. For both methods, the nucleation of islands is the phenomenon that produces an epitaxial film. Island growth introduces an unwanted defect, namely the planar arrays of threading dislocations produced when islands coalesce. In addition, a metastable crystal structure is

first observed when  $\text{Pb}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$  films are produced via the Chemical Solution Deposition method; its transformation to the stable, perovskite structure leads to rapid epitaxy and the introduction of different defects that require much higher temperatures to eliminate. Both the threading dislocation problem and the metastable phase problem are being studied by growing films on substrates that have been systematically prepared to contain well-annealed islands. This project will provide fundamental insight into a new thin film synthesis route. The synthesis of single-crystal thin films via solution methods is important to but currently absent at LANL. It will therefore provide an important complement to LANL's expertise in chemical vapor deposition, metal-organic chemical vapor deposition, molecular beam epitaxy, sputtering and laser ablation deposition. The theoretical and simulation tools at LANL will also aid in the experimental investigation to be performed at UC Santa Barbara. This project will calibrate and enhance LANL modeling capabilities as they apply to surface growth at high and low density, ferroelectric thin films, the effects of disorder and temperature on metastable precursor phases, the role of dislocations, etc.

During the overgrowth (epitaxy) of  $\text{PbTiO}_3$  (PTO) thin films on  $\text{LaAlO}_3$  (LAO) single crystal substrates it was discovered that the large lattice mismatch (4 %) between the two materials had a profound effect. The first effect was that the films were not truly epitaxial, but were a mixture of oriented grains and unoriented grains. Second, when single islands of PTO were grown on LAO, the shape (cubes) and orientation of these islands were very different from those produced when PTO islands (truncated pyramids) were produced on  $\text{SrTiO}_3$  (STO) with the much smaller lattice mismatch of 0.15 %. An equilibrium stability diagram, developed by determining the effect of different surface energies on the equilibrium shape of single crystal islands, the lowest free energy conditions for different island configurations, showed that this difference was due to the larger interfacial energy between PTO

and LAO. The second effect of the large lattice mismatch was that the PTO films produced on LAO substrates were only highly oriented polycrystalline films and not single crystals. It was shown that very good single crystal thin films of PTO could be grown on LAO substrates when the substrates were first 'seeded' with PTO single crystal islands. Once the substrates were seeded, another PTO thin film was deposited and then annealed. Using this seeding process, the epitaxial PTO thin films produced had smooth surfaces that were unobtainable when PTO thin films were deposited on the unseeded LAO substrates. The islands formed in the first step act as seeds for the growth of epitaxial thin film in the second step.

## Presentations

1. J.H. Kim, C.D.E. Lakeman, J.S. Speck, and F.F. Lange, "Formation of Epitaxial  $\text{PbTiO}_3$  Islands on  $\text{LaAlO}_3$  and  $\text{SrTiO}_3$  Substrates by Chemical Solution Deposition," Ceramic Processing '97, UC Santa Barbara, Santa Barbara, CA, September 7-10, 1997 (invited).
2. J.H. Kim and F. F. Lange, "Seeded Epitaxial Growth of  $\text{PbTiO}_3$  Thin Films on (001)  $\text{LaAlO}_3$  Using Chemical Solution Deposition Method," Materials Research Society Fall Meeting '97, Boston, MA, December 1-5, 1997 (contributed).
3. J.H. Kim, Y.S. Son, and F.F. Lange, "Stable Configuration of Epitaxial  $\text{PbTiO}_3$  Islands in Perovskite Substrates," Materials Research Society Fall Meeting '97, Boston, MA, 1-5 December 1997 (contributed).

## **9753(4) Macroscopic Ordering of Silicate-surfactant Mesophases by Electrophoresis**

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### **Abstract**

There is increasing interest in the production of new highly-ordered composite materials with novel mechanical, optical, magnetic, electronic, and/or catalytic properties. In nature, highly regular mineralized micro-laminate composites are formed through the concerted action of mechanisms that direct the organization of inorganic and organic structures over a large range of different length scales. This is not easily done using conventional synthesis techniques. For this reason, we have proposed a hybrid approach to explore strategies to create nano- to macro-scale structural order in new synthetic composite materials. One aspect of this approach involves the combination of the following two capabilities: 1) our current capabilities in the nano- and mesoscale ordering of organic molecules (surfactant) with inorganic species (silicates and analogs), and 2) the macroscopic ordering that has been demonstrated in certain systems under conditions of nonlinear dynamic control of key

properties. This project focuses on the macroscopic ordering of silicate-surfactant liquid crystal mesophases through the application of electric and magnetic fields. In the initial phases of the work, we have 1) developed appropriate nuclear magnetic resonance (NMR) hardware for *in situ* solution-phase  $^{29}\text{Si}$  NMR studies of silicate-surfactant systems; 2) obtained preliminary results indicating the presence of a silicate solution species of particular interest, a double four-membered ring (D4R) silicate, and determined its diffusion coefficient; and 3) demonstrated that aqueous silicate solution equilibria under highly alkaline conditions are not perturbed by incorporation in an agarose gel. We are now in a position to determine the electrophoretic mobility of the D4R species, that is, the diffusivity of these anions in the presence of an electric field. This will allow us to determine the effective charge on D4R for the first time. This information is needed for the development of electrophoretic processing strategies for increased structural control and patterning of inorganic-organic composite materials.

### **Refereed Publication**

1. M.D. Mann, H.L. Dai, T.A. Zawodzinski, and B.F. Chmelka, "Self-Diffusivity of Silicate Anions in Alkaline Solutions and Liquid Crystals," *Langmuir*, (in preparation).

## **9753(5) Investigation of Electron Transport Through Organic Self Assembled Monolayers Using Ballistic Electron Emission Microscopy**

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## **Abstract**

Electronic transport in organic and biomolecular materials will be one of the major thrust areas in condensed matter physics in the next century. The basic physical processes in these materials have a number of common themes. The materials have strong electron-lattice and electron-electron interactions and are disordered. They are quite different than the crystalline solids on which most efforts in condensed matter physics have concentrated until now. The phenomenology of these soft condensed matter materials is more complex and richer than that of more conventional crystalline materials. It is important to understand these kind of materials because they occur in a wide variety of important physical systems. From a technological point of view, electronics based on organic materials is an emerging field of major importance. Organic electronic materials can be economically processed over large areas and therefore they have important advantages for large area electronic applications such as displays.

Certain organic molecules have been shown to form two dimensional ordered monolayer arrays on the surface of specific metals when a film of the metal is immersed in a solution containing the molecules. These ordered monolayer films have been named self assembled monolayers (SAMs). In this project, which started in June 1997, we are investigating electrical transport through SAMs of organic molecules using ballistic electron emission microscopy (BEEM). There is

strong coupling between electronic and lattice motion in conjugated organic materials and this coupling strongly influences important physical processes such as electrical transport. Understanding such processes is beginning to have technological consequences because these conjugated organic materials are becoming important electronic materials used in, for example, organic light emitting diodes. The lattice relaxation around an electronic charge in these materials is nonlinear and not well described by the adiabatic approximation. Traditional solid state physics and quantum chemistry approaches are not adequate for an understanding of the electronic processes in these materials and new methods must be developed. SAMs can provide a well characterized model system for the study of electrical transport in conjugated organic materials. BEEM is a technique able to provide a controlled and variable energy distribution of electrons impinging on a metal/SAM interface and can be used to study the transmission of this electron distribution through the SAM film. BEEM has been shown to be an important technique for the investigation of electrical transport in inorganic materials but has not been previously used in organic materials. We are initiating a series of measurements in a well characterized experimental situation which should provide a benchmark for the development of the new theoretical methods necessary to describe electronic processes in conjugated organic systems. A graduate student, Can Zheng, has started to work on this project. During the first three months of the project she has learned the technique of BEEM and has built a dedicated apparatus for studying organic self assembled monolayers.

## **9755 Satellite Imaging Spectrometry**

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*Postdoctoral Fellow: P. Villeneuve (LANL)*

*Graduate Students: E. Collins, M. Gardner, T. Painter, and P. Sutton: (UC Santa Barbara).*

### **Abstract**

Imaging spectrometry, through near continuous sampling of the electromagnetic spectrum, represents a new technology which will significantly contribute to our abilities to detect and map trace chemical substances in the land, water and atmosphere using airborne or spaceborne remote sensing instruments. These capabilities are expected to be invaluable as tools for the detection and mapping of environmental contaminants derived from industrial and natural sources, or as byproducts from the production of biological, chemical or nuclear weapons. The tools that are being developed within this project for analyzing imaging spectrometry data are expected to contribute significantly to the environmental sciences, for example through the understanding of pollution pathways, and to the prevention of the proliferation of weapons of mass destruction, such as nuclear or biological weapons, for

example by means of the early detection of proliferation attempts. Several mapping techniques have already been developed for minerals, trace gases and chemical constituents over the past decade. However, most of these techniques were developed for analysis of data from developmental airborne sensors and have only been applied to relatively small data sets.

Our research partnership was initiated in March 1997 to combine the complementary strengths of the Los Alamos and UC Santa Barbara teams in order to gain experience with the analysis of hyperspectral images, i.e., images obtained over a large number of spectral channels. The partnership also works together on characterizing spectral signatures of interest for non-proliferation and environmental assessments, and in developing new analysis tools for imaging spectrometry. We identified and prioritized 13 potential collaboration topics and started sharing common data sets such as spectral libraries and hyperspectral images from a new developmental instrument, the Spatially-Enhanced Broad band Array Spectrograph System (SEBASS). Currently, these data sets are used in the application of detection and identification algorithms to locate chemical constituents in an atmospheric plume over variable land background.

### **Refereed Publication**

1. D.A. Roberts, R.O. Green, and J.B. Adams, "Temporal and Spatial Patterns in Vegetation and Atmospheric Properties from AVIRIS," *Remote Sens.*, 62, 223 (1997).

### **Non-Refereed Publications**

1. D.A. Roberts, M. Gardner, R. Church, S.L. Ustin, and R.O. Green, "Optimum Strategies for Mapping Vegetation using Multiple Endmember Spectral Mixture Models," *Proceedings of the International Society for Optical Engineering (SPIE), Imaging Spectrometry III (Descour, M.R., and*

*Shen, S.S. Eds.), 3118(14), 108 (1997).*

2. T. H. Painter, D.A. Roberts, R.O. Green, J. Dozier, "Estimating Snow Cover and Grain Size from AVIRIS Data with Spectral Mixture Analysis and Modeled Snow Spectra," *Proceedings of the International Society for Optical Engineering (SPIE), Imaging Spectrometry III (Descour, M.R., and Shen, S.S. Eds.), 3118(14), 120 (1997).*

### Presentations

1. C.C. Borel, "Iterative Retrieval of Surface Emissivity and Temperature for a Hyperspectral Sensor," First Jet Propulsion Laboratory Workshop on Remote Sensing of Land Surface Emissivity, Pasadena, CA, May 6 - 8, 1997 (contributed).

2. J. Theiler and G. Gisler, "Contiguity-Enhanced k-Means Clustering Algorithm for Unsupervised Multispectral Image Segmentation," International Society for Optical Engineering (SPIE) Conference 3159 on Algorithms, Devices, and Systems for Optical Information Processing, San Diego, CA, July 27 - August 1, 1997 (contributed).

3. D.A. Roberts, M. Gardner, R. Church, S.L. Ustin, and R.O. Green, "Optimum Strategies for Mapping Vegetation Using Multiple Endmember Spectral Mixture Models," International Society for Optical Engineering (SPIE) Conference 3118 on Imaging Spectrometry III, San Diego, CA, July 27-August 1, 1997 (contributed).

4. T.H. Painter, D.A. Roberts, R.O. Green, and J. Dozier, "Estimating Snow Cover and Grain Size from AVIRIS Data with Spectral Mixture Analysis and Modeled Snow Spectra," International Society for Optical Engineering (SPIE) Conference 3118 on Imaging Spectrometry III, San Diego, CA, July 27 - August 1, 1997 (contributed).

## **9759 A Mesoscopic Optical Instrument for Detection of TNT**

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*Graduate Student: Carlos Gonzalez (UC Davis).*

### Abstract

The goal of this project is to demonstrate a prototype, miniature, chemical sensing module, which can detect and measure the selective adsorption of gas phase molecules using optical sensing techniques. The test case species for detection will be TNT and other explosives. Selective adsorption is achieved by the attachment of highly sensitive and selective ultrathin films to the surface of planar optical waveguides. The sensing module is built in and on a micromachined silicon, optical breadboard, implementing a set of new micro-machined structures that enable the modular assembly and alignment of the optical and sensing components. A key feature of the module is that the planar optical waveguides can be removed, coated, analyzed in other types of instruments, and replaced into the instrument.

Miniaturized, smart sensor array systems are needed to address a variety of national security and civilian problems. The need is especially acute for rapid, point detection of chemical or biological agents and in the detection of land mines. Species selective thin

films for molecular recognition and self-assembly techniques for attachment to sensor surfaces have been under development at the Los Alamos National Laboratory for several years. Current research is centered on the development of Zeeman interferometry and related optical transduction techniques that are capable of very high sensitivity. But, traditional optical metrology requires expensive, rather bulky components. For field applications, a flexible, light weight, cost effective, yet highly precise instrument is required. Silicon based micro-instruments can meet these requirements due to the batch nature of their manufacturing and photolithographically defined geometries. However, until recently, the assembly of micro-instruments was piece-meal, labor intensive and unalterable. The new assembly technology in development at UC Davis solves this problem. The success of this project will revolutionize analytical instrument design and development in general, and produce a highly sensitive, yet cost effective, instrument for field testing of the highly selective films and optical detection schemes under investigation at Los Alamos. The ultimate result will be a small, low cost, light-weight, smart instruments that can be sent into mine fields on remote controlled vehicles. The highly collaborative and interdisciplinary nature of this research project provides a rare training opportunity for graduate students and a special opportunity for researchers at UC Davis to apply newly developed technology to socially relevant, highly challenging, real world engineering problems.

Commercially obtained laser diodes, optical fibers, and planar optical waveguides have been mounted on silicon micro-machined stages, and assembled onto a silicon breadboard for alignment and testing. Components are mounted on orthogonal x and yz micro-stages. At this time, alignment is performed by moving the stages manually with a micromanipulator probe. Preliminary experiments have demonstrated butt coupling of laser light from the end of an optical fiber into the planar waveguide. The assembly will soon be shipped to Los Alamos for optical testing and evaluation.

## **9760 Improved Measurements of the Newtonian Gravitational Constant**

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### **Abstract:**

The work performed by Los Alamos under this program centers on the fabrication of large copper rings to be used by R. Newman at UC-Irvine. The role of Los Alamos is to supply certified copper material that has been machined and inspected to very close tolerances. Dr. Newman came to Los Alamos because of our extensive experience in close tolerance machining and inspection. The rings will be used in an experiment to determine the gravitational constant. Recent published work has shown a wide variation in the calculated Newtonian gravitational constant based on different experimental techniques. The work by R. Newman will use a well established experiment to confirm the gravitational constant. The accuracy of the experiment will rest solely on the detailed fabrication of the copper rings.

## **9761 Los Alamos National Laboratory/UC Irvine Bridge & Ground Vibration Testing Project**

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*Undergraduate Student: Jose Valles  
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### **Abstract**

UC Irvine personnel collaborated with Los Alamos National Laboratory personnel on the ambient and forced testing of the 8-span Alamosa Canyon bridge north of Truth or Consequences, New Mexico during the week of July 21 to July 25, 1997. Of particular interest to the UC Irvine team were the bridge and ground vibration tests that determined the bridge's vertical direction modal properties with UC Irvine's seismic shaker and the bridge's lateral direction modal properties using an eccentric mass shaker, which quantified the ground vibration and soil-structure interaction levels at test locations along and perpendicular to the bridge deck.

UC Irvine and Los Alamos personnel used similar multi-channel, HP 3565 dynamic signal analyzers and PCB 393C accelerometers. In addition to Los Alamos' data acquisition/data reduction hardware/software capability and its hammer and truck excitation techniques, UCI contributed its hardware and expertise to the Los Alamos project with (a) its 30 lb. and 100 lb. APS seismic shakers, (b) the UCLA and/or UCI eccentric mass shaker, (c) 8-12 UCI/UCLA seismometers, (d) HP3562, HP35665, HP3565 dynamic signal analyzers, and (e) PCB accelerometers.

The bridge superstructure vibration response data has been incorporated into LANL's Damage Detection software (DIAMOND). The ground vibration data will provide UCI with experimental data to complement its analytical soil dynamic model.

## **9762 Technologies for Imaging Brain Function**

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*Undergraduate Student: Maurizio Di Mauro  
(University of New Mexico).*

### **Abstract**

The purpose of this project, under way for a little more than one month, is to strengthen interactions and collaborations between the laboratories of Ron Harper of the Brain Research Institute at UC Los Angeles, and John George of the Biophysics Group at Los Alamos National Laboratory. These laboratories have developed special expertise in complementary areas of brain functional mapping.

The specific aims of this project include the development of a new imaging probe for optical measurement of neural function. The initial version of this device will be configured as a miniature endoscope, allowing access to deep brain regions via a gradient index relay lens cylinder that can be less than a

millimeter in diameter. This device can be configured for confocal or spectral imaging according to a design by George that is the subject of a LANL/UC patent application. In order to optimize this system for brain functional imaging we plan to pursue the development of an advanced CCD imager, and a high-performance data acquisition and control subsystem.

The second area of collaboration will be in the development of methods for human brain mapping for application to scientific problems of interest to both laboratories. Harper and colleagues are developing experimental methods for functional MRI studies of the processes regulating respiration and cardiac cycle. George and colleagues are working on the technological basis of such measurements, including implementation of a large bore research imager, development of software for analysis, and development of methods for physiological monitoring inside the magnet bore.

2. R.F. Rogers, D.M. Rector, R.M. Harper, J.S. Schwaber, , and J.S. George, "Light Scattering Change from the Dorsal Brainstem during Pressor Challenges and Spontaneously Evoked Activity," *Society for Neuroscience meeting, New Orleans, LA, October 25-31,1997* (contributed).

3. J.S. George, "Dynamic Neuroimaging: Integrating MRI, fMRI, & MEG," *Society for Neuroscience Meeting, New Orleans, LA, October 25-31,1997* (invited).

## Patents

1. J.S. George, "Scanned Computed Confocal Imager," US patent pending.

## Non-Refereed Publications

1. D.M. Rector, R.F. Rogers, and J.S. George, "A Compact Endoscope Imaging System for Neural Activity Assessment In-Vivo," *Society for Neuroscience Abstracts, 23, 840* (1997).

2. R.F. Rogers, D.M. Rector, R.M. Harper, J.S. Schwaber, and J.S. George, "Light Scattering Change from the Dorsal Brainstem during Pressor Challenges and Spontaneously Evoked Activity," *Society for Neuroscience Abstracts, 23, 840* (1997).

## Presentations

1. D.M. Rector, R.F. Rogers, and J.S. George, "A Compact Endoscope Imaging System for Neural Activity Assessment In-Vivo," *Society for Neuroscience Meeting, New Orleans, LA, October 25-31,1997* (contributed).



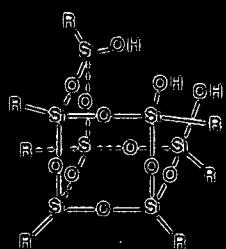
## Investigator Index for UCDRD Projects

In this index, we have listed the principal investigators from Los Alamos and the UC campuses for the UCDRD projects described in this report with reference to the page numbers where their project abstracts can be found. Additional collaborators, postdoctoral fellows, and students are not included.

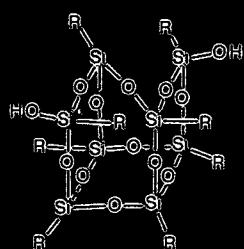
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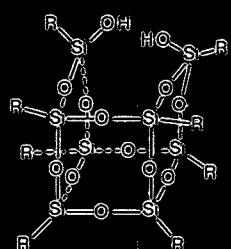
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Yu, Clare (UCI), 80  
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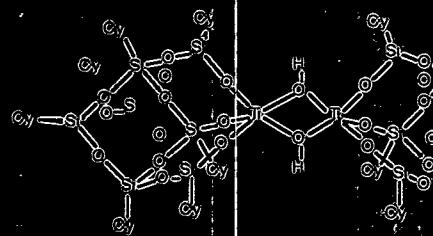
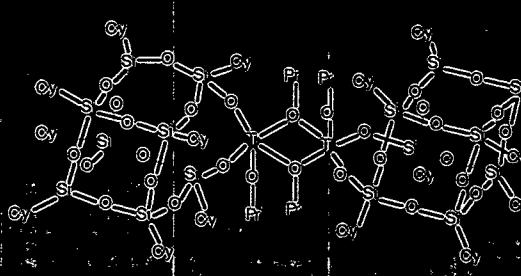
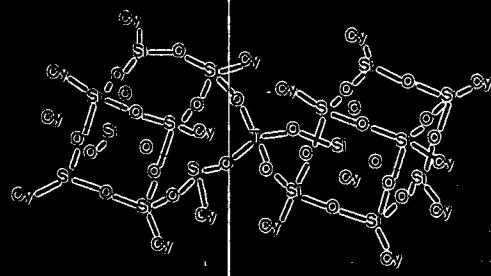
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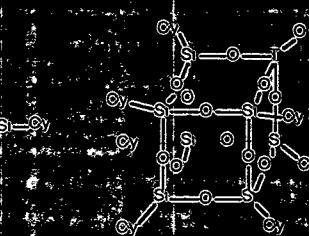
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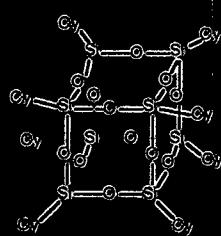
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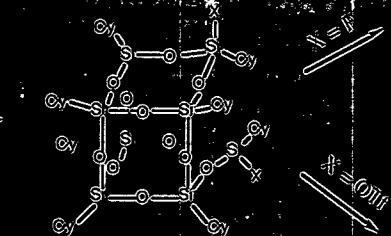
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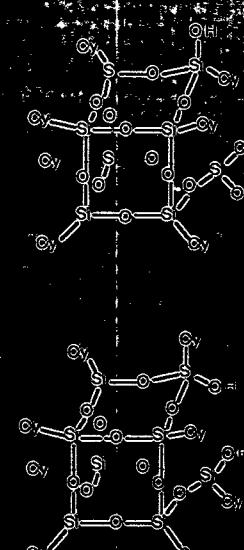
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## **Appendix A: CULAR Program Call for Proposals**

### **Collaborative UC/Los Alamos Research (CULAR) Proposals Due: Spring 1998**

#### **Purpose**

The CULAR program funds joint research projects between the Los Alamos National Laboratory and University of California (UC) Campuses that enhance the Laboratory's competencies in selected areas and that strengthen the technical ties between the Laboratory and the Campuses.

#### **Program Description and Duration of Project Funding**

A research project is jointly proposed by a Los Alamos Investigator (LI) and a Campus Investigator (CI) in one of the following Technical Focus Areas:

- Bioscience and Biotechnology
- Earth and Environmental Systems
- Materials Science

Funding requests may not exceed \$55k per year. Most of the funding should be spent by the Campus, but at least 10% must be spent by Los Alamos. A new proposal can describe work to be performed over a period not to exceed 3 years, but approval for funding will be granted one year at a time. This Call is soliciting proposals for work to be funded for the period of October 1, 1998 to September 30, 1999 (Laboratory Fiscal Year 1999).

#### **Additional Proposal Guidance**

The proposed research should be collaborative and should build on the complementary personnel capabilities and research facilities of Los Alamos and the Campus. One goal of the CULAR program is to allow campus participants to become more familiar with Los Alamos capabilities and facilities. To this end, the research is to be carried out at Los Alamos or at both Los Alamos and the participating Campus. In the latter case, Campus participants should spend a portion of the project time working at Los Alamos. Graduate student participation is encouraged, but limited to students who have completed their course requirements and are in the research stage of their degree requirements.

The proposal format and instructions follow.

## **Proposal Submission and Review Process**

The first step of the proposal review and selection occurs at the Campus under the direction of the Campus Research Administrator (e.g., Vice Chancellor for Research). No more than 4 new (first-year) proposals may be submitted per year by a given Campus. All continuing (second- and third-year) proposals from a Campus may be submitted. The method of reviewing and selecting proposals at the Campus is left up to the Research Administrator, but the process should ensure that the proposals meet all of UC requirements including the approval by the Campus contracts and grants office. One copy of the selected proposals (new and continuing) must be submitted no later than May 22, 1998 to:

UC Coordinator  
MS F673  
Los Alamos National Laboratory  
Los Alamos, NM 87545

The LI and CI have the responsibility for meeting the campus deadline for submission. Each campus will have its own submission date and selection process prior to the May 22 deadline at Los Alamos.

The Laboratory UC Coordinator will give the new proposals to a Los Alamos technical review committee for the Technical Focus Area selected by the proposal LI and CI and listed on the Data Sheet. The technical review committee will provide a written evaluation and numerical score based on the evaluation criteria listed below. The numerical scores from this evaluation will be used to rank the new proposals.

## **Proposal Evaluation Criteria**

- Creativity and innovation (30)
- Technical impact (on the scientific field in general and on the Laboratory and Campus capabilities) (30)
- Feasibility (20)
- Importance of complementary capabilities and facilities at the Campus and Laboratory to carry out the proposed research (20)

The continuing (second- and third-year) proposals will be given a scientific management review by the UC Coordinator to ensure that reasonable technical progress has been made and that the quality of collaboration is fulfilling the purpose of the CULAR Program. Subject to the availability of UC-DRD funds, these proposals will usually continue to be funded if they pass this management review. However, if a continuing proposal requests a larger budget than was granted the first year, that proposal will be treated like a new proposal (except that the earlier year(s) will count against the 3-year limit) and will be counted as 1 of the 4 new campus submissions. Because the probability of continued funding is substantially less in this case, requesting larger budgets for the second and third year is not recommended.

Based on the above reviews and rankings and the requested budgets in each proposal, the UC Coordinator will select the proposals to be funded and the budget level for each proposal. Contingent on the availability of funds, up to 10 new proposals will be selected, in addition to the continuing projects. The LIs and CIs will be notified of these decisions by August 21, 1998.

## **Proposal Format and Instructions**

*The proposal consists of four main parts:*

Data Sheet  
Body  
Budget Sheet  
Attachments.

## 1. Data Sheet

The quality and completeness of the information on this page can strongly influence the initial ranking of the proposal during the technical review process. The length of the Data Sheet must not exceed one page and must not contain fonts smaller than 12 point (the size used in this set of instructions). The LI and CI can determine which technical committee reviews their proposal by entering the desired Technical Focus Area on the Data Sheet. If the designation of either the LI or CI as Principal Investigator is desired, enter "PI" or "Principal Investigator" after the appropriate name on both the Data Sheet and the first page of the proposal.

The figures in the funding profile table should be the sum of the proposed budgets for the Campus and the Laboratory. The total of both operating and capital should not exceed \$55K per year. As explained in the Proposal Submission and Review Process section, it is recommended that the budgets requested in the second and in the third year not exceed that requested in the first year.

*The format of the Data Sheet is:*

Los Alamos National Laboratory  
FY 1999 CULAR Data Sheet

Project Title:

Los Alamos Investigator (LI):

Group:

Address:

Telephone:

Email:

Campus Investigator (CI):

Campus:

Address:

Telephone:

Email:

Technical Focus Area: *(Select one of the 3 listed in the Call)*

Nature and Significance of Proposed Work:

Previous Year's Major Accomplishments  
*(If applicable):*

Work Proposed for FY 1999, Goals, and  
Expected Results:

CULAR Funding Profile:

Fiscal Year:

FY 1999

FY 2000

FY 2001

Operating (k\$):

Capital (k\$):

Total (k\$):

## 2. The Body

The body of the proposal can be no greater than 5 pages in length using fonts no smaller than 12 point. The text on the Data Sheet (not included in the 5-page limit) is considered the abstract for the proposal and therefore no other abstract is desired in this document.

*The format of the body of the proposal follows:*

### FY 1999 CULAR Project Proposal

Project Title:

LI Name:

CI Name:

LI Address:

LI Email:

CI Address:

CI Email:

Background and Rationale:

Research Objectives and Goals:

Technical Impact:

Research Approach:

Technical Progress Summary: (For second- and third-year proposals only) (Limit to 1 page including list of publications, conference papers, patents, awards, and degrees derived from this CULAR-funded work. Also include the names of the postdocs and graduate students that worked on this activity.)

Expected Technical Results:

Capabilities at the Campus and Los Alamos: (Include both facilities and expertise.)

Literature Cited:

## 3. Budget Sheet

The portions of these expenditures to be made by the Campus and the Laboratory should be listed separately. The Campus expenditures should be more than half of the budget, but at least 10% should be spent by the Laboratory. Show all direct costs for FY 1999 only, including salary, benefits, materials and services, equipment, and travel. Make sure the sum of the Campus and Laboratory costs agrees with that on the Data Sheet.

The CULAR Program is a DOE Laboratory (Los Alamos National Laboratory) University of California Collaborative Activity. The costs of this Program will be paid entirely from UCDRD funds. These are University funds held in an account at the UC Office of the President (UCOP). These funds will be transferred by Los Alamos direction directly to the UC Campus for the Campus expenditures. Because UCDRD funds are University funds, they are deemed to be intramural and therefore not subject to A-21 overhead rates. Proposals from Campus faculty must be submitted through their contracts and grants office for the usual approvals.

Funds for Los Alamos expenses will be transferred to the appropriate Los Alamos group. No G&A burden will be imposed by the Laboratory.

It is in the interest of the Laboratory to encourage support of collaborative activities; therefore, campus budgets may include, at the option of the campus research administrator, an amount of up to ten percent of the total direct Campus costs for this purpose. This will be a lump amount intended to be retained by the Office of the Vice Chancellor for Research. This lump amount to support collaborative activities is a program objective and is not to be interpreted as in lieu of indirect costs, since indirect costs are not required under this program. The lump sum is a direct cost, and should be labeled "Campus/Los Alamos Collaborative Activities Support" in the Budget Sheet.

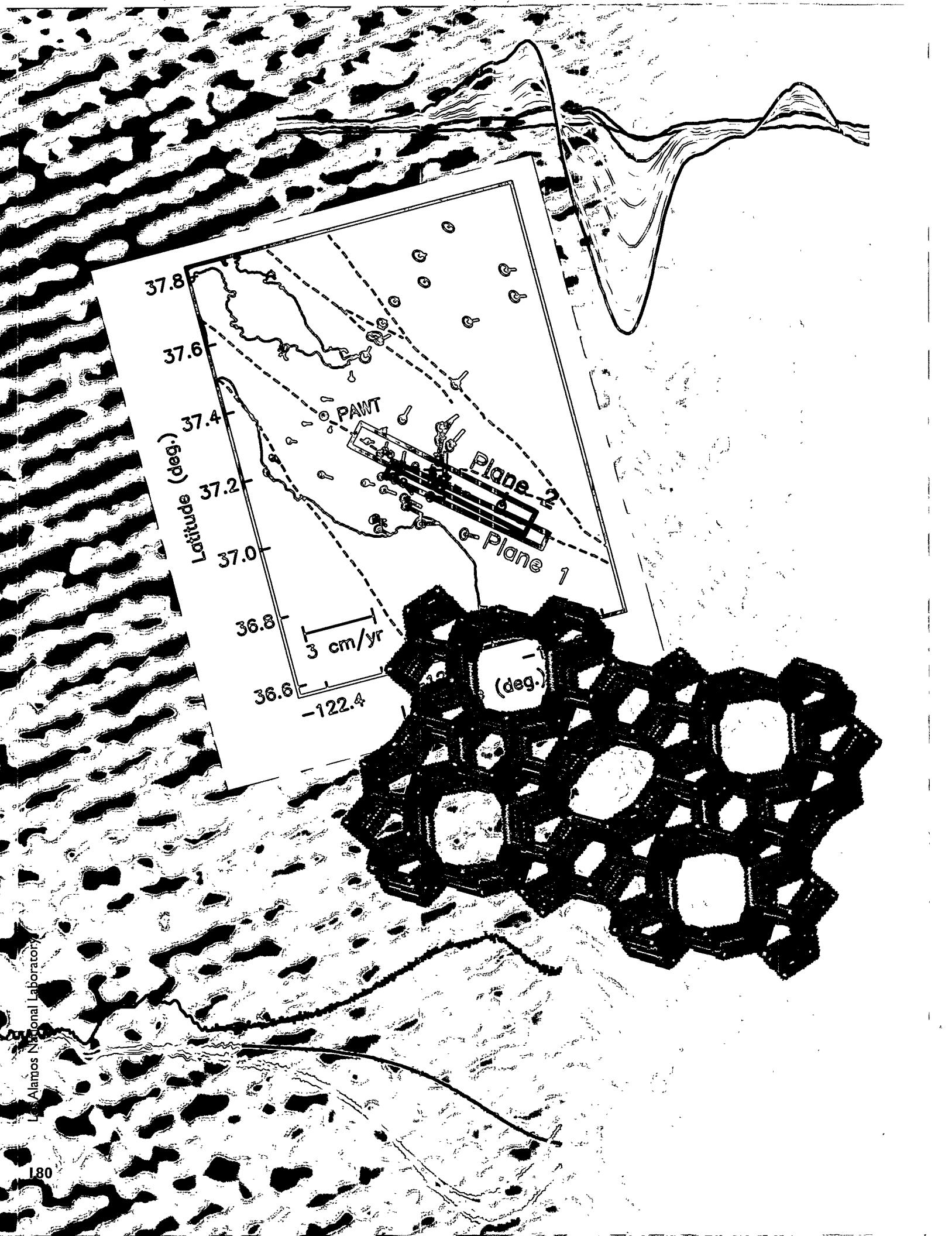
#### **4. Attachments**

The following must be attached to the proposal:

A. Curriculum Vitae (Attach 1-page vitae for the LI, CI, and other major participants. Include only the most important publications that pertain to the proposed work.)

B. Required Documentation (All required documentation to comply with University, Campus, Laboratory, and DOE requirements including those associated with ES&H and living subjects (human or animal) compliance.)

UC/LANL Collaborative UC/Los Alamos Research Call for Proposals



## **Appendix B: Visiting Scholar Program Call for Proposals**

**Proposals Due: February 10, 1997**

### **Purpose**

The Visiting Scholar Program funds Los Alamos National Laboratory staff to do research and related teaching at a University of California (UC) Campus, or UC faculty to do research at the Laboratory. The intent of this program is to allow the host institution and the participant to benefit from closer professional interactions while fostering collaborative research between the Campus and the Laboratory. Participants will be competitively selected for these appointments based on the criteria outlined in this Call.

### **Program Description and Eligibility**

The Program will fund the salary and associated expenses (described below) of the participant while carrying out research and related activities at a proposed location for a period between 6 months and 1 year. Eligibility is restricted to UC faculty who are members of the Academic Senate or to regular Los Alamos technical staff members. UC faculty who are not US citizens are fully eligible and a lack of security clearance should not impede research activities at Los Alamos in the majority of cases.

The awards will be announced in May 1997. Regardless of the beginning date, the proposal should be for a continuous period of 6 months to 1 year. The funds currently available for this Call will allow the support for only four to eight awards total (Campuses plus Laboratory).

### **Funding**

The funds for the Visiting Scholar Program come entirely from the Los Alamos portion of the University of California Directed Research and Development (UCDRD) account. The funds will be supplied to the home organization (UC campus for faculty, and Los Alamos group for Laboratory staff) so that paychecks, benefits, etc., will continue unaltered from the normal process.

In general, funding will be provided for salary (including summer salary for faculty), benefits, travel, some off-site living expenses, and a small amount for research equipment, materials, and services. Some portion of the funds for materials and services could be sent to the host institution if that is deemed useful by the Visiting Scholar. Detailed requests should be included in the budget sheet attached to the proposal as described later in this Call.

## **Proposal Submission and Selection Process**

The proposal, including required attachments, must be received at the following address no later than February 10, 1997:

Dr. Rulon K. Linford  
UC Coordinator  
MS F673  
Los Alamos National Laboratory  
Los Alamos, NM 87545

The format and instructions for all elements of the required proposal are attached.

No limitation is imposed on the number of proposals submitted from a given Campus department or Laboratory group. However, applicants should consider the competitive selection criteria and the maximum number of awards to be made before making the effort to apply.

These proposals will be evaluated by peer reviewers and then ranked by the Selection Committee comprised of Vice Chancellors for Research, faculty chosen by the Academic Council, and Los Alamos National Laboratory Fellows or Senior Fellows, and chaired by the Los Alamos UC Coordinator. The peer reviewers will individually score the proposals according to the following evaluation criteria. Using the input from the peer reviewers, the members of the Selection Committee will individually develop their own scores using the same evaluation criteria, and then rank the proposals. (Vice Chancellors for Research and faculty will not score proposals from their own Campus and Fellows will not score proposals from their own Division.) Then during a conference call or meeting of the Committee the candidates will be discussed and a final selection will be made.

## **Evaluation Criteria (maximum points for each criterion)**

- Quality of proposed research (creativity of approach, potential impact on technical field, and feasibility of proposed work). (50)
- Benefit to the Laboratory and the Campus (strengthened collaboration, capabilities, skills, contact with students, and opportunities for increased external/extramural funding; for Laboratory staff going to a campus, importance of teaching opportunity should be included). (30)
- Importance of complementary capabilities and facilities available at the selected Campus/Lab to carry out the proposed research. (20)

The awards will be announced in May 1997. These appointments could begin as soon after the announcements as the details could be worked out. Practical considerations would probably prevent most appointments from beginning before June 1997. As stated above, the latest start date for this round will be June 26, 1998. Regardless of start date the appointments will be for a continuous period of 6 months to 1 year.

## **Proposal Format and Instructions**

The proposal consists of six main parts: the Body, the Curriculum Vitae, the Budget Sheet, the Letter of Support from Applicant's Supervisor, the Letter of Support from the Host Organization, and the list of four suggested peer reviewers.

## 1. The Body

The Body contains two parts: the title block (see format below) and the main body. Both of these parts must be contained within four pages and must not contain fonts smaller than 12 point (the size used in this set of instructions). The main body should contain a description of the research and teaching activities being proposed, the anticipated results and their importance to the technical field, and the benefits to both the Campus and the Lab. (See the evaluation criteria.) In addition, the main body should indicate the importance of the capabilities and facilities that the applicant will have access to at the host institution in carrying out these activities. The main body should also contain a brief statement about the adequacy of support (beyond that requested on the attached budget sheet) needed for other elements of the collaboration.

The format of the title block for the Body of the proposal is:

### Proposal for Visiting Scholar Program

#### Applicant Data

Name:

Dept./Group:Address:

Telephone:Supervisor:

(Department Chair, Group Leader, etc.)

Telephone:

#### Host Institution Data

Principal Collaborator:

Dept./Group:Address:

Telephone:Collaborator's Supervisor:

(Department Chair, Group Leader, etc.)

Telephone:

#### Appointment Data

Dates of Desired Appointment:Beginning:

Ending:Total Requested Budget  
(from Budget Sheet):

Title or Topic of Research/Teaching:

## 2. Curriculum Vitae

The CV should be restricted to one, or two pages at the most. Only the most important publications that are relevant to the proposed research/teaching activity should be included.

## 3. Budget Sheet

Show all direct costs including salary, benefits, materials and services, travel, and off-site living expenses. The off-site living expenses should be consistent with the relevant campus travel policies or the Laboratory's Extended Travel Guidelines. These expenses will include housing, transportation, and per diem. To minimize unnecessary work, the applicant should use an estimate of \$3000 per month for the off-site living expenses (housing, local transportation, and per diem). The details will be negotiated later with those who are selected to take into account the location and other special circumstances. The result may be somewhat lower or higher than this estimate. In addition to the travel at the beginning and end of the appointment, travel expenses can include round-trip airfare that can include trips to relevant scientific conferences and allows the applicant to return to the home institution no more frequently than every six weeks. We actually recommend that the applicant return periodically for a few days to maintain appropriate contacts. It may be useful to allocate a small amount of funding to be made available to the Visiting Scholar at the host institution for materials and services. If this is desired, please indicate the amount as part of the budget sheet.

The Visiting Scholar Program is a DOE Laboratory (Los Alamos National Laboratory) University of California Collaborative Activity. As stated earlier, the costs of this Program will be paid entirely from UCDRD funds. These are University funds held in an account at the UC Office of the President (UCOP). These funds will be transferred by Los Alamos direction directly to the UC campus for faculty that are selected for an award without flowing through Los Alamos. Because UCDRD funds are University funds, they are deemed to be intramural and therefore not subject to A-21 overhead rates. Funds for Los Alamos staff that are selected for an award will be transferred to the appropriate Los Alamos group. No G&A burden will be imposed by the Laboratory. Proposals from Campus faculty must be submitted through their contracts and grants office for the usual approvals.

It is in the interest of the Laboratory to encourage support of collaborative activities, therefore budgets for faculty may include an amount up to ten percent of total costs, at the option of the Campus for this purpose. This will be a lump amount intended to be retained by the Office of the Vice Chancellor for Research. This lump amount to support collaborative activities is a program objective and is not to be interpreted as in lieu of indirect cost, since indirect costs are not required under this program. This amount should be labeled "Campus /Los Alamos Collaborative Activities Support" in the Budget Sheet.

#### **4. Letter of Support from Applicant's Supervisor**

This letter should indicate that the supervisor (e.g., Department Chair or Group Leader) is supportive of the proposed activity and that the impact of the applicant's absence can be adequately managed. In particular, a Laboratory supervisor should provide assurance that the applicant will have a job when the appointment is over, and a Campus supervisor should indicate that the ap-

plicant's teaching responsibilities can be covered and that the appointment will at least not hurt the applicant's status in the Department. The letter should be brief. While a simple statement of recommendation is appropriate, it is not intended that this letter contain a detailed assessment of the applicant's qualifications.

Letters of support that are written by Laboratory Group Leaders should be in the form of a memo sent through the cognizant Division Director. This letter of support should indicate the willingness of the group and division to initiate a Personnel Action Form financially transferring the Laboratory Visiting Scholar to the STB-UC organization for the length of the visit. (This transfer is accomplished by putting the STB cost center in the "Proposed Status" cost center box and leaving the "Organization Code" box blank, thus the Visiting Scholar administratively remains in their present group.) This change avoids group and division taxes while the Visiting Scholar is away from the Laboratory.

#### **5. Letter of Support from the Host Organization**

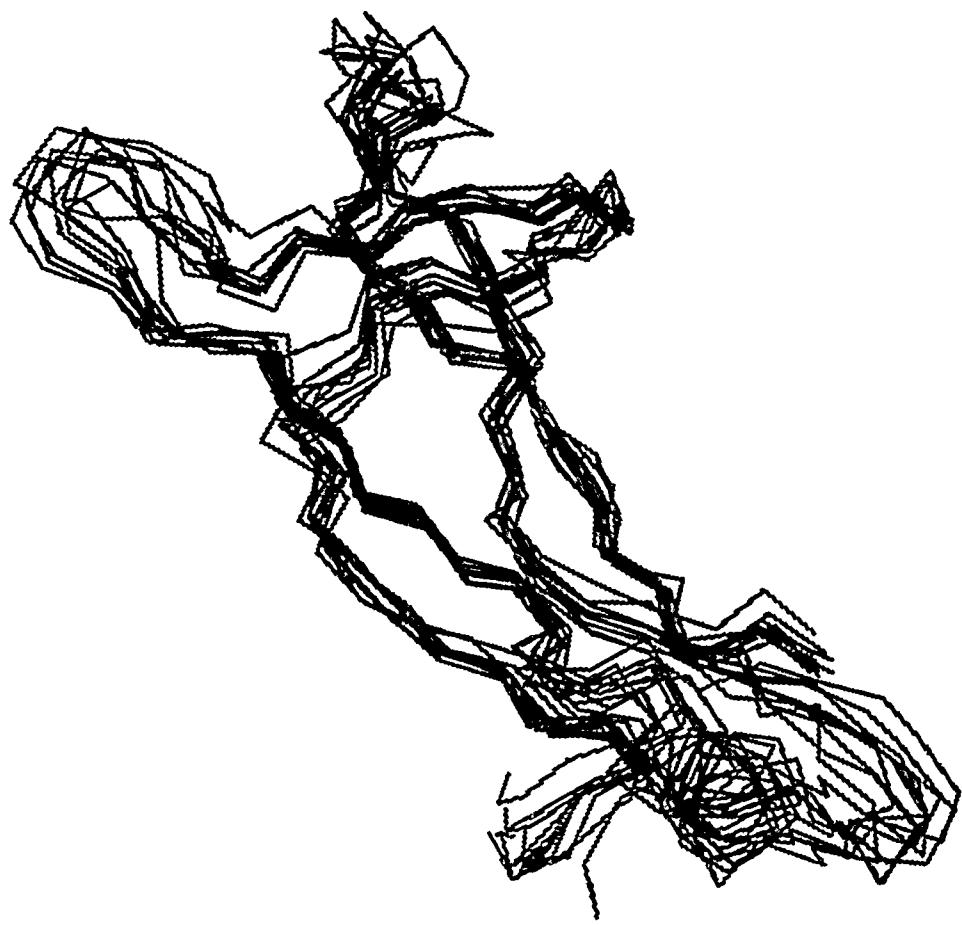
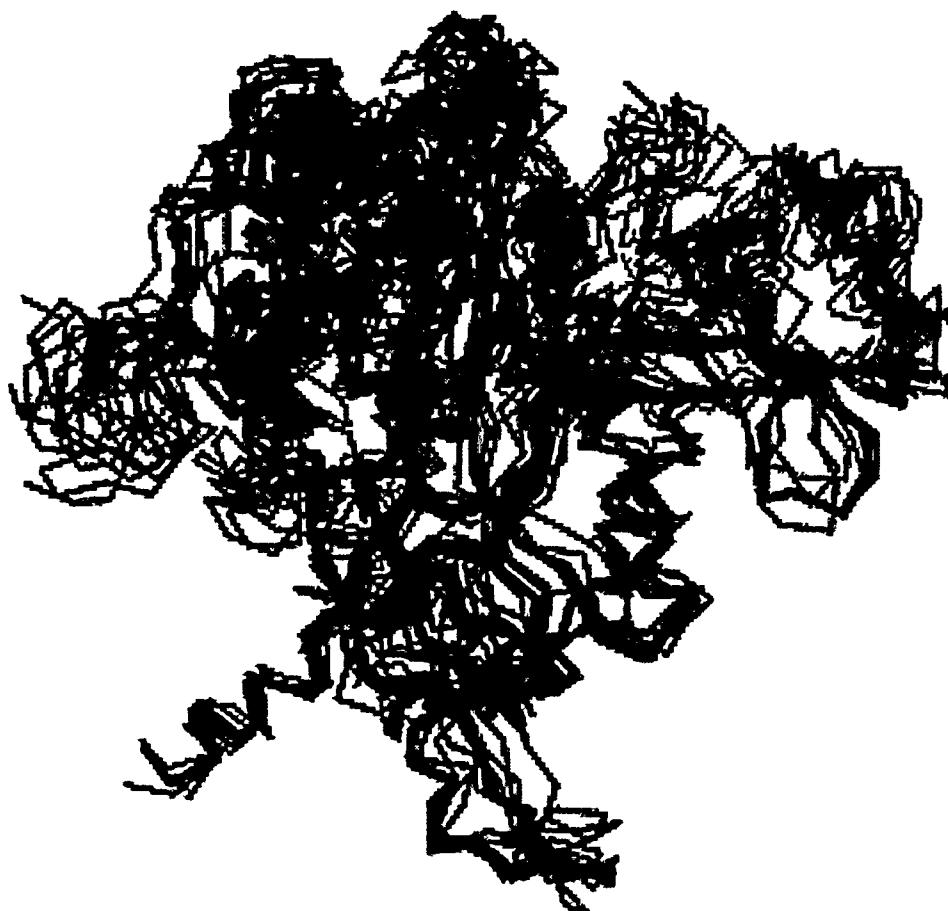
This letter should be written by the supervisor (e.g., Department Chair or Group Leader) of the applicant's principal collaborator at the host institution. It should indicate support for the applicant's proposal and that the visit can be accommodated by the organization. Specifically, a Laboratory Group Leader should indicate that office and lab space and other appropriate facilities and needs can be provided. A Department Chair should indicate that the proposed teaching by the applicant is appropriate and that adequate office and research space and other appropriate facilities and needs are available. A brief statement of recommendation is also appropriate, but no detailed assessment of the applicant's qualifications is expected.

Letters by Laboratory Group Leaders should be in the form of a memo sent through the cognizant Division Director. The letter should state that the hosting group will submit a Guest Scientist Agreement and oversee the necessary Laboratory training and regulations for a guest scientist. Letters from the Department Chair should indicate the official status within their department and campus of the Visiting Scholar, (i.e., Senior Researcher, Researcher, etc.) Such a designation may be useful for the individual to have appropriate access to campus services and have the ability to access appropriate budgets for materials and supplies as described in (3) Budget Sheet above.

The proposed research activities must comply with all of the pertinent University, Campus, Laboratory and DOE requirements. In particular, any required special documentation regarding ES&H and living subjects should also be attached to the proposal.

#### 6. List of Peer Reviewers

Please provide a list of four suggested researchers who could provide a peer review of the proposal. They obviously should have no conflict of interest in regards to the proposal. Please include name, institution, address, phone number, fax, and email.



# **Appendix C - Application Procedures for Los Alamos National Laboratory - University of California (UC) Campuses Research Partnership Initiatives**

## **Purpose**

The Research Partnership Initiatives foster the development of research collaborations between Los Alamos and one or more UC campuses in areas of strategic interest to the Laboratory. An important goal is to assist these initiatives to become strong programs sustained by funds from external customers.

## **Program Description and Eligibility**

The Research Partnership Initiatives provide seed funding for collaborative research in areas of strategic interest to Los Alamos that have potential for external support in the future. The proposed research should build on the complementary personnel capabilities and research facilities of Los Alamos and the Campuses. While the overall collaboration may involve institutions outside of UC, only UC campuses and Los Alamos National Laboratory are eligible to receive Research Partnership Initiative funding. There is no formal call for proposals and no specific deadline. When funding becomes available, white papers that have been received will be considered.

## **Funding**

The funds for the Research Partnership Initiatives come entirely from the Los Alamos Portion of the University of California Directed Research and Development (UCDRD) account. The amount of funding for new Initiatives from year to year depends on commitments to continuing projects, unallowable costs at the Laboratory, and changes in the UC contract with DOE for managing the Laboratory. Only small amounts are likely to be available for new Initiatives during the remainder of FY 1998.

## **Application Submission and Selection Process**

An informal proposal should be submitted by email or mail in the form of a one- or two-page white paper to:

Dr. James C. Porter  
UC Coordinator  
MS F673  
Los Alamos National Laboratory  
Los Alamos, NM 87545  
[porter@lanl.gov](mailto:porter@lanl.gov)  
Phone: (505) 665-0736  
Fax: (505) 665-3199

The quality of the proposed research (creativity of approach, potential impact on technical field and feasibility of the proposed work), its strategic value to the Laboratory, and the potential for the collaboration to attract external funding will be evaluated by the UC Coordinator when funds become available. If the project is selected for some level of support, the UC Coordinator will request a more formal proposal and budget information.

### **Application Format**

A one- to two-page white paper should be submitted containing the following information:

Title of the Collaboration,

Names and affiliations of main participants,

Description of the research being proposed,

Anticipated results,

Benefits to the Campuses and the Laboratory,

Potential for external funding in the future, and

Budget estimate. (List the total estimated cost by year for each institution for the duration project. No indirect costs at the Campus or G&A burden at the Laboratory should be included.)

### **Selected Proposals**

If a proposal is selected, the UC Coordinator will contact you for a more complete proposal with an itemized budget sheet. University funding will require submittal by the campus contract and grants office. The following budget sheet will give guidance on this submission.

### **Budget Sheet for Research Partnership Initiatives UCDRD Funded Activities**

The portions of expenditures for the Campus and the Laboratory should be listed separately. The Research Partnership Initiatives is a DOE Laboratory (Los Alamos National Laboratory) University of California Collaborative Activity. The costs of this program will be paid entirely from UCDRD funds. These are University funds held in an account at the UC Office of the President (UCOP). These funds will be transferred by Los Alamos direction directly to the UC Campus for the Campus expenditures. Because UCDRD funds are University funds, they are deemed to be intramural and therefore not subject to A-21 overhead rates. Proposals from Campus Faculty must be submitted through their contracts and grants office for the usual approvals.

Funds for Los Alamos expenses will be transferred to the appropriate Los Alamos Group. No G&A burden will be imposed by the Laboratory.

It is in the interest of the Laboratory to encourage support of collaborative activities; therefore, campus budgets may include, at the option of the campus research administrator, an amount of up to ten percent of the total direct Campus costs for this purpose. This will be a lump amount intended to be retained by the Office of the Vice Chancellor for Research. This lump amount to support collaborative activities is a program objective and is not to be interpreted as in lieu of indirect costs, since indirect costs are not required under this program. The lump sum should be labeled "Campus/Los Alamos Collaborative Activities Support" in the Budget Sheet.

## **Appendix D Call for Proposals**

### **New Mexico Universities Collaborative Research (NUCOR)**

#### **Academic Year 1998-1999**

#### **Proposals Due: March 6, 1998**

##### **Purpose**

The NUCOR program funds joint research projects between the Los Alamos National Laboratory and four New Mexico universities (New Mexico Highlands, New Mexico State, New Mexico Tech, and University of New Mexico). Projects are funded that enhance the Laboratory's competencies in selected areas and that strengthen the technical ties between the Laboratory and the Universities.

##### **Program Description and Duration of Project Funding**

A research project is jointly proposed by a Los Alamos Investigator (LI) and a University Investigator (UI) in one of the following Technical Focus Areas:

- Satellites and Remote Sensing
- Earth and Environmental Systems
- Materials and Advanced Manufacturing

Funding requests may not exceed \$55k per year. More than 50% of the funding should be spent by the Universities, but at least 10% must be spent by Los Alamos. A new proposal can describe work to be performed over a period not to exceed 3 years, but approval for funding will be granted one year at a time. The sole source of support for the NUCOR Program is the Los Alamos portion of the University of California Directed Research and Development (UCDRD) funds. Continued funding for the second and third year will, in part, depend on the availability of these funds which varies from year to year. This Call is soliciting proposals for work to be funded for the period of August 15, 1998 to August 14, 1999. This period is referred to as "Academic Year 1998-99" in this Call for Proposals.

##### **Additional Proposal Guidance**

The proposed research should be collaborative and should build on the complementary personnel capabilities and research facilities of Los Alamos and the Universities. Participants in the project are expected to spend a significant portion of the project time at Los Alamos and the participating University so that they become familiar with the resources at all of the institutions involved in the project. Graduate student participation is encouraged, particularly those who have completed their course requirements and are in the research stage of their degree requirements. NUCOR support of graduate students who are still taking courses should be restricted to the fraction of their time devoted to the proposed research. Support for undergraduate students can be sought by submitting a supplemental request for up to \$10k per proposal for non-NUCOR funds.

This document is available in three data formats. These include HTML, Adobe Acrobat PDF and Microsoft Word. Adobe Acrobat PDF is a platform independent file format for distributing documents. Adobe provides information on the WWW on how to obtain free Adobe Acrobat PDF Reader software and other Adobe product information. An Adobe Acrobat PDF version of this document is available from this WWW site.

The proposal format and instructions follow.

### **Proposal Submission and Review Process**

The first step of the proposal review and selection occurs at the University under the direction of the Research Administrator or by a person designated by the University. No more than 4 new (first-year) proposals may be submitted per year by a given University. All continuing (second- and third-year) proposals from a University may be submitted.

The method of reviewing and selecting proposals at the University is left up to the Research Administrator or University designee, but the process should ensure that the proposals meet all of the University requirements including the approval by the contracts and grants office. One copy of the selected proposals (new and continuing) must be submitted no later than March 6, 1998 to:

STB-UC Coordination Team  
MS F673  
Los Alamos National Laboratory  
Los Alamos, NM 87545

The new proposals will be evaluated by peer reviewers and then ranked by a technical review committee for the Technical Focus Area selected by the LI and UI as listed on the Data Sheet. The peer reviewers will individually score the proposals according to the evaluation criteria listed in the following paragraph. Using the input from the peer reviewers, the members of the technical re-

view committee will individually develop their own scores using the same evaluation criteria, and then rank the proposals. (Technical review committee members will not score proposals from their own division.) Then during a conference call or meeting of the committee the candidates will be discussed and a final selection will be made.

### **Proposal Evaluation Criteria**

- Creativity and innovation (25)
- Technical impact (on the scientific field in general and on the Laboratory and Campus capabilities) (20)
- Feasibility (20)
- Qualifications of the LI, UI, and other technical participants for this task (15)
- Importance of complementary capabilities and facilities at the University and Laboratory to carry out the proposed research (10)
- Reasonableness of budget, schedule, and facilities for completing the proposed work (10)

The continuing (second- and third-year) proposals will be given a scientific management review by the UC Coordinator to ensure that reasonable technical progress has been made and that the quality of collaboration is fulfilling the purpose of the NUCOR Program. Subject to the availability of UCDRD funds, these proposals will usually continue to be funded if they pass this management review. However, if a continuing proposal requests a larger budget than was granted the first year, that proposal will be treated like a new proposal (except that the earlier year(s) will count against the 3-year limit) and will be submitted to the appropriate technical review committee. Because the probability of continued funding is substantially less in this case, requesting larger budgets for the second and third year is not recommended.

Based on the above reviews and rankings and the requested budgets in each proposal, the UC Coordinator will select the proposals to

be funded and the budget level for each proposal. The supplemental requests for non-NUCOR funds associated with the selected proposals will be reviewed by the Team Leader for University Programs. These requests will be granted on the basis of the additional strength brought to the project and the availability of funds. The LIs and UIs will be notified of these decisions by June 22, 1998.

The figures in the funding profile table should be the sum of the proposed NUCOR budgets for the University and the Laboratory. (Supplemental non-NUCOR funds should not be included here.) The total of both operating and capital should not exceed \$55K per year. As explained in the Proposal Submission and Review Process section, it is recommended that the budgets requested in the second and in the third year not exceed that requested in the first year.

## **Proposal Format and Instructions**

The proposal consists of five main parts:

1. Data Sheet
2. Body
3. Budget Sheet
4. Attachments.
5. Supplemental Request for Non-NUCOR Funds (Optional)
6. List of Peer Reviewers

### **1. Data Sheet**

The quality and completeness of the information on this page can strongly influence the initial ranking of the proposal during the technical review process. The length of the Data Sheet must not exceed one page and must not contain fonts smaller than 12 point (the size used in this set of instructions). The LI and UI can determine which technical committee reviews their proposal by entering the desired Technical Focus Area on the Data Sheet. If the designation of either the LI or UI as Principal Investigator is desired, enter "PI" or "Principal Investigator" after the appropriate name on both the Data Sheet and the first page of the proposal.

The format of the Data Sheet is:

Los Alamos National Laboratory  
Academic-Year 1998-99  
NUCOR Data Sheet

Project Title:

Los Alamos Investigator (LI):

Group:

Email:

Address:

Telephone:

University Investigator (UI):

University:

Email:

Address:

Telephone:

Technical Focus Area: (Select one of the 3 listed in the Call)

Nature and Significance of Proposed Work:

Previous Year's Major Accomplishments (If applicable):

Work Proposed for Academic Year 1998-99, Goals, and Expected Results:

NUCOR Funding Profile:

Academic Year:

1998-1999  
1999-2000  
2000-2001

Operating (K\$)  
Capital (K\$)  
Total (K\$)

page including list of publications, conference papers, patents, awards, and degrees derived from this NUCOR-funded work. Also include the names of the postdocs and graduate students that worked on this activity.)

Expected Technical Results:

Capabilities at the Universities and Los Alamos:

(Include both facilities and expertise.)

## 2. The Body

The body of the proposal can be no greater than 5 pages in length using fonts no smaller than 12 point. The text on the Data Sheet (not included in the 5-page limit) is considered the abstract for the proposal and therefore no other abstract is desired in this document.

The format of the body of the proposal follows:

Academic-Year 1998-99 NUCOR Project Proposal

Project Title:

LI Name:

UI Name:

LI Address:

UI Address:

Background and Rationale:

Research Objectives and Goals:

Technical Impact:

Research Approach:

Technical Progress Summary: (For second- and third-year proposals only) (Limit to 1

Literature Cited:

## 3. Budget Sheet

The expenditures to be made by the Universities and the Laboratory should be listed separately. The total university expenditures should be more than half of the budget, but at least 10% should be spent by the Laboratory. Show all direct costs for Academic Year 1998-99 only (August 15, 1998 to August 14, 1999), including salary, benefits, materials and services, equipment, and travel. Materials and equipment will be owned by the institution (University or DOE (Laboratory)) making the purchase. Make sure the sum of the University and Laboratory costs agrees with that on the Data Sheet.

The costs of the NUCOR Program will be paid entirely from UCDRD funds. These funds are held in an account at the UC Office of the President and will be transferred by Los Alamos direction directly to the NM Universities for the University expenditures. No indirect costs at the Universities will be paid, but up to \$5k of administrative support of the research at the University will be allowed as a direct cost on each proposal. Proposals from University faculty must be submitted through their contracts and grants office for the usual approvals.

Funds for Los Alamos expenses will be transferred to the appropriate Los Alamos group.

No G&A burden will be imposed by the Laboratory.

University:

Address:

Telephone:

#### 4. Attachments

The following must be attached to the proposal:

A. Curriculum Vitae (Attach 1-page vitae for the LI, UI, and other major participants. Include only the most important publications that pertain to the proposed work.)

Description of Undergraduate Involvement: (Include type of work student(s) will be doing and how much time each student will be working, e.g., one student 20% during academic year and full time during summer, second student 70% time during summer.)

B. Required Documentation (All required documentation to comply with NM University, Laboratory, and DOE requirements including those associated with ES&H and living subjects (human or animal) compliance.)

Impact of Undergraduate Contributions: (Describe the importance of the undergraduate student involvement to the success of the project.)

Supplemental Budget Sheet: (Provide the budget information that is required by the University contracts and grants office for the support of the undergraduate students. Indirect costs are not allowed.)

#### 5. SUPPLEMENTAL REQUEST FOR NON-NUCOR FUNDS (OPTIONAL)

The Supplemental Request should be limited to one or two pages. No more than \$10k can be requested per year for involvement of undergraduate students with the associated NUCOR project. The format for the request is provided below.

#### 6. List of Peer Reviewers

Please provide a list of three suggested researchers who could provide a peer review of the proposal. They obviously should have no conflict of interest in regards to the proposal. Please include name, institution, address, phone number, fax, and email.

Last updated on Thursday, December 18, 1997.

Academic-Year 1998-99

Supplemental Request for Non-NUCOR Funds

Project Title: (Same as the associated NUCOR proposal)

Los Alamos Investigator (LI):

Group:

Address:

Telephone:

University Investigator (UI):