Director’s Statement

2011-12 has been a busy and successful year for NEAT, as the achievements highlighted in this newsletter attest. Our international collaborations continue to blossom, with strong ties to China, Brazil, Israel and elsewhere. I, Gang-Yu Liu, and several other UCD faculty attended a workshop on chemical biology at the Chinese Chemical Society meeting in Chengdu, Sichuan China and enjoyed the science, wonderful food, and hospitality. I am expanding collaborations with Sichuan University, both in our joint “111” program emphasizing environmental science and in chemistry and materials science, with an exchange scholar coming this fall. I also visited the Three Gorges Dam and impounded Yangtze River upstream of it, viewing both a remarkable engineering achievement and serious environmental and social challenges. Our Brazilian connections are expanding. Professor Ricardo Castro, originally from Sao Paulo, Brazil, and now faculty in Chemical Engineering and Materials Science and of the NEAT ORU and Peter A. Rock Thermochemistry Laboratory, received tenure and a promotion to associate professor effective July 1, 2012. His Ph.D. adviser, Professor Douglas Gouvea, is spending a sabbatical with us and a student of his is also spending a year here. Brazil anticipates sending a large number of students to the U.S. for graduate education and UC Davis has signed a formal agreement of cooperation with Brazilian agencies. I plan to visit Brazil this August. We expect more great science and wonderful barbecues to ensue. I visited Israel in June, where we have an expanding cooperation with Ben-Gurion University (see photo).

Research in NEAT is progressing well. In addition to our two EFRCs and ICAM, Giulia Galli and I are involved in a large Sloan Foundation project, the Deep Carbon Observatory, which seeks to understand the geochemical carbon cycle not just at the Earth’s surface but throughout the planet. Bill Casey’s work, with several new grants, links the geochemical behavior of transition metals in minerals and aqueous clusters with the catalysis of water splitting in a materials and energy context. In addition, much new equipment has been purchased an installed, see below.

We have had significant staff changes. Gladis Lopez has left to be MSO of the math department, and Ruth Victor has succeeded her. A second analyst, Marlene Mooshian, has been hired to help Shanna Nation Jose manage proposals and grants. Our part time and student help keeps changing. Our goal is to provide exemplary service in proposal and grant management to our entire NEAT faculty who process grants through our office; please let me and/or Ruth know how we can serve you better.
ICAM - THE INSTITUTE FOR COMPLEX ADAPTIVE MATTER

The scientific investigation of physical and biological systems requires that we not only study the properties of the pieces, but also search for the organizing principles behind the emergent behavior of the systems. Emergence reminds us that you are not going to solve a scientific problem just by looking at the parts. Leading us into the frontiers of a new science of emergence, the Institute for Complex Adaptive Matter (ICAM) is an open distributed experiment-based dynamic multi-institutional partnership. ICAM's purposes are: to identify major new research themes in complex adaptive matter; to nucleate and conduct collaborative research and scientific training that links together scientists in different fields and different institutions; and to convey the excitement breakthroughs in the physical and biological sciences to young scientists and the general public through education and outreach. ICAM's areas of investigation are (i) Quantum matter, including strongly interacting electrons in metals and cold atoms in magnetic traps, (ii) biological matter - such as self-assembled protein aggregates in viral capsids or Alzheimer's disease victims, (iii) soft matter - like liquid crystals and lipid bilayers which mimic cell membranes.

As an institute without walls, ICAM's growth has been tremendous within the past year. We welcome Piers Coleman as ICAM's new co-director, alongside Daniel Cox. Dr. Coleman is replacing someone who is irreplaceable—the founding director of ICAM, David Pines. “Becoming Engaged: Initiatives That Can Change Science Education-An ICAM/ Aspen Center for Physics 50th Anniversary Workshop” (to be held in July) commemorates Dr. Pines’ commitment to starting ICAM/I2CAM and seeing the Institute through to maturity. His choice was to favor a workshop on science engagement to honor his I2CAM/ICAM legacy.

As a distributed scientific institute, ICAM is expanding its integrated scientific and educational programs.

New Branches

The ICAM/I2CAM network has maintained its size with many new possible branches in the offing. We have added branches in the form of a consortium of University of Denver/Colorado School of Mines/Univ. Colorado Denver, a consortium in Parma, and the Center for Materials & Microsystems/Bruno Kessler Foundation in Trento, Italy. We have three new branches ready to join in the summer at Northeastern University, Argonne National Labs, and the Superconductivity Research Frontier Center of Brookhaven/Illinois/Cornell. We are also in discussion with possible new branches at the University of Arkansas, in the UK, and Singapore.

A significant development was our support for two workshops and a school in Argentina (the school also held sessions in Uruguay). We are thus expanding our strong presence in Brazil to other parts of South America as well. Our biggest single initiative is to work with our colleagues in China to develop an ICAM-China network with comparable funding to I2CAM and with an expansion by a factor of three of our branches in China. The proposal to the Chinese government for this is in place. This will enable far more collaborations between China and the US, but also between ICAM-China and other branches around the world.

Education

ICAM's expanding educational role includes exploratory workshops, schools for junior scientists, fellowships, travel awards for junior scientists, and education outreach efforts. The past year has seen 33 new publications resulting from I2CAM sponsored research, workshops, and schools, and 7 PhD dissertations.

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Overall, 1575 junior and 1185 senior scientists have participated in I2CAM related activities in the past year, representing more than 10 different disciplines in science and engineering. I2CAM has, with the help of leveraging, supported 5 schools, our annual conference, and 24 workshops/conferences in ICAM related science. These workshops have covered such topics as pattern formation in biology, nonequilibrium quantum systems, nanoscale materials building blocks, and ferroelectric liquid crystals. The schools have covered advanced photonic materials, topological insulators, methods for modern electronic structure computation, transition metal oxide materials, and quantum impurity physics. The workshop on disordered superconductors generated a multinational grant within Europe being considered for funding by the European Union.

I2CAM continues to expand its library of online lectures from our workshops and the Boulder Condensed Matter Summer School. At present, we have uploaded 671 presentations to the ICAMVID channel on SciVee.Tv, with over 41,300 viewings of the archived lectures. The superconductivity wing of ICAM's emergentuniverse.org online museum is now open. As part of the superconductivity wing, with support from our branch contribution fund, our museum designer Suzi Tucker commissioned a “flash mob” dance representation of superconductivity, which became viral on youtube.com.

What's next?

In the period from now through next Fall Year, ICAM has current plans to provide support to 22 workshops and 7 schools in addition to our usual support for individual exchange awards and travel awards for junior scientists. This includes the planned school on sustainable energy being held in Boulder. The plan is to hold this in Boulder, to seek co-organization with staff from the National Renewable Energy Laboratory, and to see if we can have partial synergy with the annual Boulder School on Condensed Matter Physics through a few days of shared lectures and mutual activities for the students. If the meeting is successful we plan to hold it every year in Boulder. In addition, there is considerable interest in developing an annual school in China.

**SCIENCE, EDUCATION, ENGAGEMENT (SEE): NEW INITIATIVE AND COURSES**

Professor Alexandra Navrotsky and Professor David Pines, with the help of consultant Steve Hartzog, created and taught two new multidisciplinary courses during Winter Quarter 2012. Professors Navrotsky and Pines created the courses after recognizing the nationwide need for defining and developing the science and technology of sustainability, a discipline that combines “the fundamental and applied research we need to make proposed ‘Clean Energy’ technologies economically competitive”. The two courses, “Gateways to Emergence in Science and Society” and “The Internet as a Medium for Education about Science and Sustainability”, aimed to unite a diverse group of scientists, artists, and educators behind the joint effort of creating an emergent strategy for improving science education on sustainability.

Students in the “Internet as a Medium” course, taught by Steve Hartzog, collaborated on the creation of a new online resource intended to enrich and advance science education for the key demographic of 11-18 year old students and their teachers. While in its sister course, “Gateways to Emergence” taught by Professors Navrotsky and Pines, students focused on sustainability-related research and its importance to the future generations.

Throughout the quarter, Professors Navrotsky and Pines enlisted the help of a number of internal and external distinguished colleagues who are world leaders in their respective fields. These individuals were invited to spend two days on campus, during which they gave a major public lecture one evening and met with the Emergence students the next morning during class meeting.

Overall, the courses were a great success. Students, faculty, and visiting lecturers alike enjoyed the courses and called for their continuation. Emergence will be taught again in Winter 2014 by Professors Navrotsky and Zimanyi.
To visit the Emergence Course site, please visit, http://emergence.ucdavis.edu/. For recordings of the guest lectures, please visit the UCTV Seminars page, http://seminars.uctv.tv/, and sort by UC campus.

**PETER A. ROCK THERMOCHEMISTRY LABORATORY** *(Professors Navrotsky & Castro)*

After 40 years of building unique calorimeters, Professor Navrotsky’s “workhorse” oxide melt solution calorimeter has been commercialized by Setaram Inc. as the AlexSYS. One has been installed in the Peter. A. Rock Thermochemistry Laboratory and is so reliable that even a dog can use it (seriously it works very well). A user workshop on the AlexSYS was held in Davis this June.

- Laser evaporation chamber is in operation with 100 W CO2 laser and being used for synthesis of oxide nanoparticles.
- New system including 400 W CO2 laser, aerodynamic levitator with split nozzle and splat quenching is funded by Office of Naval Research and in construction
- Ultra-high temperature thermal analysis instrument (Setaram Setsys) was upgraded for operation up to 2500 °C.
- Two Setaram C-80 calorimeters for analyses from 25 to 300 °C. These very sensitive instruments are employed to measure heat of solution, heat of immersion in both organic solvents and aqueous solutions. They are used for in situ synthesis calorimetry as well.
- Setaram C-80 calorimeter with appropriate cells coupled with Teledyne ISCO syringe pump system for calorimetric measurements at high pressure, up to 300 bar.

**SPECTRAL IMAGING FACILITY**

The NEAT ORU Spectral Imaging Facility is a recharge based user facility on the UC Davis campus, located in Chemistry Rm 11, offering a state-of-the-art atomic force microscope combined with a laser scanning confocal microscope, a field emission scanning electron microscope, and a Raman microscope to the research community supporting investigation and research in the multi-disciplined fields of Bio-Nano and Nano-Materials. A development engineer specialized in materials characterization, nano-technology, and bio imaging is available daily to assist users with training and use of the microscopes and to assist with sample preparation.

The microscopes available to users include:

The state-of-the-art high-resolution Asylum Research, Inc. MFP-3D versatile atomic force microscope capable of imaging samples in liquid as well as air while sharing the IX-81 microscope sample stage with the Olympus America FV1000 laser scanning confocal microscope. The FV1000 system has six laser lines and 4
spectral channels including bright-field for sample imaging, the Hitachi High Technologies America, Inc. S-4100 FE-SEM (Field Emission Scanning Electron Microscope) with Quartz PCI SlowScan digital image capture system provides micrographs of samples using acceleration voltages of 500 to 30k Volts where resolution approaches 1.5 nm. An Oxford Instruments, Inc. INCA Energy EDS (Energy Dispersive X-ray Spectrometry) is attached to the S-4100 for elemental X-ray microanalysis from element Boron on up, and the Renishaw RM1000 Raman microscope with upgrades for 2D Raman spectra using either Argon 514 nm or diode 785 nm lasers and epi-fluorescence.

The FORMA 1460 Biological Safety Cabinet and NAPCO incubator are available to users for the benefit of live-cell imaging while using the microscopes in the facility.

The Spectral Imaging Facility is supported by recharges to University of California researchers and affiliates at nominal rates for both Assisted and Unassisted microscope use. Users may submit samples for imaging or complete the microscope user training and become a Certified User with the associated benefit of unassisted access at the lower recharge rate. Also available for general use is a dedicated computer workstation affording image analysis of acquired data.

Please contact the development engineer for the facility, Alan Hicklin (sif-info@ucdavis.edu), for details regarding training, scheduling, and advice on sample preparation.

**EQUIPMENT AND FACILITIES NEWS**

**Charles Fadley**  
Professor Fadley’s group is close to completing the upgrading of a quick turnaround XPS facility in the Physics Department that will soon be available on a recharge basis for routine surface analysis.

**Gang-Yu Liu**  
Professor Liu’s group has completed a state-of-the-art apertureless near-field scanning optical microscope (NSOM) that is made available to collaborators at NEAT ORU. The intrinsic advantages of this approach include: (a) high photon throughput with the ability to tune wavelength; (b) simplicity in detection of near-field optical signals because the PL exhibits different wavelength from the excitation beam; (c) high spatial resolution due to the apertureless AFM platform with sharp probes and effective deflection feedback; and (d) simplicity in operation.

**Susan Kauzlarich**  
Professor Kauzlarich’s group recently acquired the Linseis LSR3 which is used for measuring Seebeck Coefficient / Electric Resistance from room temperature to 1100˚C.

**STUDENT AND POSTDOC ACCOLADES**

**Donglei Bu**, a graduate student from the Liu group, received a 2011 Graduate Research Award as well as a 2011 ICAM Travel Award to attend the 242nd ACS Meeting in Colorado for a poster presentation.

**Randy Dumas**, a postdoctoral researcher from the Liu group, was awarded the Young Researcher Award by the Swedish Research Council in 2011 for his work on magnetic materials.

**Tako Endo**, from the Sen group, received a 2-year fellowship from Japan Society for Promotion of Science to work on dynamics in glass-forming room temperature ionic liquids

**Dustin Gilbert**, a graduate student from the Liu group, was selected by the IEEE Magnetics Society to participate in its 2012 Summer School at Sri Ramaswamy Memorial University in Chennai, India.

**Peter Greene**, a postdoctoral researcher from the Liu group, was elected to be a 2012 NSF EAPSI Fellow which allows him to attend the East Asia and Pacific Summer Institutes at the National Tsing Hua University in Taiwan.

**S.Mahboobeh Hosseini**, a Ph.D student from the Navrotsky group, started the Materials Research Society
chapter at UC Davis in 2011; she is now president of the chapter. She was also awarded 2011 Best Poster at the Annual Board of Advisors Meeting for the CEMS department at UC Davis in addition to earning the Student Award at the 18th Solid State Ionics Society Conference in Poland, July 2011.

Sixiao Hu, a Ph.D student from the Hsieh group, was awarded the grand prize at the National Textile Center Forum for the paper titled “Mesoporous ultra-high specific carbon nanofibers from lignin”.

Jie-Ren Li received a 2011 ICAM Travel Award to attend the 242nd ACS Meeting in Colorado for a poster presentation.

Chengcheng Ma, a Ph.D student from the Navrotsky group, was awarded the 2011 GSR Summer Fellowship from Graduate Study at UC Davis.

Greg McAlpin, a graduate student from the Casey group, was awarded Best Dissertation in 2012, which is the top award given to graduate students in the Chemistry department.

Thomas Myers, a postdoctoral researcher from the Berben group, was awarded the Volman Fellowship, for excellence in his graduate studies, in addition to the ACS Division of Inorganic Chemistry Student Travel Award for the 2012 spring meeting.

**FACULTY ACCOLADES**

Louise Berben was elected to be a 2012 Alfred P. Sloan Foundation Fellow. This two-year fellowship is awarded yearly to 118 researchers in recognition of distinguished performance and a unique potential to make substantial contributions to their field. Professor Berben was also awarded the NSF CAREER Award, a 5 year research grant.

William Casey received the Herbert A. Young Society Dean’s Fellowship in the Division of Mathematical and Physical Sciences to be used for teaching, research, and service activities.

Ricardo Castro was awarded tenure; his promotion to Associate Professor is effective July 2012. Professor Castro received the 2011 SHPE Outstanding Young Investigator Award, given by the Society of Hispanic Professional Engineers to young scientists who have contributed to the progress of research in any field of science and engineering. Also in 2011, he received the NSF Career Award and the DOE Early Career Award, both awards are intended to support the development of outstanding scientists early in their careers. Professor Castro was also awarded the 2012 Outstanding Junior Faculty Award by the Dean of the College of Engineering.

Charles Fadley was elected to be a 2011 Fellow of the American Association for the Advancement of Science as well as a 2012 Eletta Fellow for the Italian National Synchrotron Radiation Laboratory (Elettra) for his fundamental contributions to the development of photoelectron spectroscopy, diffraction and holography worldwide. Fadley was also awarded a substantial two year grant from the French national program to promote world-class laboratories in physics (Laboratoires d’Excellence: Physique: Atomes, Lumiere, Matiere--PALM) as a visiting Distinguished Professor.

Saif Islam was awarded the 2012 Outstanding Mid-career Research Faculty Award by the Dean of the College of Engineering.

Susan Kauzlarich was elected a 2011 ACS Fellow. Kauzlarich was also awarded the IUPAC Distinguished Women in Chemistry/Chemical Engineering in 2011, the award was designed to acknowledge and promote the work of women chemists and chemical engineers worldwide. Kauzlarich also received the Iota Sigma Pi National Honorary Member Award in 2011, the award is the highest honor that Iota Sigma Pi bestows on outstanding women chemists.

Kai Liu was elected to be a Fellow at the Institute of Physics (UK), an honor that indicates a very high level of achievement in physics and an outstanding contribution to the profession.

Alexandra Navrotsky’s manuscript “Thermochemistry of Lanthana and Yttria Doped Thoria”, jointly written with Michael Aizenshtein and Tatiana Y. Shvareva, was selected to be the Featured Manuscript in the Journal of the American Ceramic Society in 2011.

Frank Osterloh received the Scialog Collaborative Innovation Award for 2012 which allows his research group to fabricate and test Fractal Shaped Solar Cells with improved performance.
Warren Pickett was elected to be a **2012 Simons Fellow** which provides him with the funds to support his sabbatical.

Pieter Stroeve was elected to be a **2012 Fellow of the American Institute of Chemical Engineers** for his contributions to the advancement of the Chemical Engineering discipline.

Yayoi Takamura received the **2011 DARPA Young Faculty Award**, an award that aims to identify and engage rising stars in junior faculty positions in Department of Defense matters.

### NEW GRANTS RECEIVED: MAY 2011 – AUGUST 2012

Here is a list of new awards given during this period:

- NASA: “Research Opportunities in Space and Earth Science (ROSES-2010), Astrobiology: Exobiology and Evolutionary Biology” **Casey**
- Department of Energy (DOE): “Adding Reactivity to Structure-Kinetics of Oxygen-Isotope Exchanges at Structural Sites in Nanometer-Size Aqueous Molecules” **Casey**
- Brown Univ subcontract, Office of Naval Research: “Rational Design of Refactory Materials: A Combined Computational and Experimental Approach” **A. Navrotsky**
- Department of Energy (DOE): “Energetics of Radiation Tolerant Nanoceramics” **R. Castro**
- National Science Foundation (NSF): “Thermochemistry of Nanoceramics: Understanding and Controlling Phase Transformation and Sintering via Interface Energetics” **R. Castro**
- UC Lab Fees (UCOP): “Design of Nanoceramics with High Radiation Tolerance” **R. Castro**
- UC Lab Fees (UCOP): “Damage Resistant Structures Fabricated by Laser Chemical Vapor Deposition for High Power Laser Optics and Photonics Applications” **G. Galli**
- National Science Foundation (NSF): “Goalsi: Structure-Property Systematics in Novel Chalcogenide Glasses with Modified Networks” **S. Sen**
- UNISANTA, Brazil: “NANOENERGY - ELEKTRO - Carbon Nanotubes Applied to the Reduction of the Technical Losses on the Energy Distribution System” **R. Castro**
- NSF EAGER: “Exploring Routes to Nanocomposites Linking Silicate and Carbon-Based Structures” **A. Navrotsky**
- Department of Energy (DOE): “Thermochemistry of Oxides with Electrochemical and Energy Applications” **A. Navrotsky**

These awards, plus the continuation of existing ones, lead to a total of $7.7 million in extramural funding in NEAT/ICAM for the current year.

### NEAT IN THE NEWS

Professor William Casey and Professor James Rustad were highlighted in a “News and Views” article by Paul Fenter in *Nature Materials*. This article discussed their advance in understanding reaction dynamics in aqueous oxides. The article received wide attention in the general-science media for synthesizing two decades worth of research into a simple model.
The essence of the result is a linkage between isotope-exchange and dissociation reactions. Both proceed via sets of low-energy intermediate states. This model explains many long-standing mysteries about aqueous reactivities. (See Figure to the right)

**Professor Gang-Yu Liu** and **Professor Ian Kennedy** were awarded $1 million by the W. M. KECK Foundation for the development of a new device to measure mechanical properties of cells, as well as activity within them. The new confocal microscope will allow one to view details of a single cell by pressing a tiny bead against it to measure resistance, enabling the testing of a wide range of cells types to study toxicity of nanoparticles. Dr. Liu’s lab has previously demonstrated the potential of the microscope concept with nerve cells and the new instrument will better enable testing to determine if mechanical properties change with early damage to live cells. 


Professor Alexandra Navrotsky’s joint review with Professors Rodney Ewing and Peter Burns was published with a cover picture in *Science* in the March 9, 2012 edition. The review, titled “Nuclear Fuel in a Reactor Accident”, addresses the March 2011 tsunami that destroyed three nuclear reactors in Japan. Their article discusses “current understanding of nuclear fuel interactions with the environment, including studies over the relatively narrow range of geochemical, hydrological, and radiation environments relevant to geological repository performance, and discuss priorities for research needed to develop future predictive models”.

Professor Alexandra Navrotsky and Dr. Sergey Ushakov were recently mentioned on the American Ceramic Society’s blog, Ceramic Tech Today. The article on Professor Navrotsky and Dr. Ushakov, titled “Hot stuff: Measuring thermophysical properties at very high temperatures”, discusses their review “Experimental Approaches to the Thermodynamics of Ceramics above 1,500°C” that was recently published in the *Journal of the American Ceramic Society*. The review discusses methods for measuring high temperature thermophysical properties, how to measure melting point, and how to determine phase diagrams in refractory systems.

**NEAT FACULTY COLLABORATIVE PUBLICATIONS 2011-12 (NEAT faculty in bold)**


“Experimental Methodologies for Assessing the Surface Energy of Highly Hygroscopic Materials: The


**Ph.D THESSES FROM RECENT NEAT GRADUATES**


NEAT BENEFACTORS: MARCH 2011 – MARCH 2012
Alexandra Navrotsky
American Superconductor
Carbon Design Innovations, Inc
Matthew Augustine
TE Connectivity
Trinity Capital Corp
UC Davis
Wolf Ridge Environmental Learning Center

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Rain does not dampen NEAT’s enthusiasm at the Solid State Ionics Meeting in Warsaw, Poland (Summer 2011)

Another year … another birthday … another party; NEAT has its cake and eats it too!