Though I highlighted last year as one of change, the 2013—2014 year has been one of rapid evolution, bringing both challenge and opportunity to NEAT and the university, and 2014—2015 promises to evolve even faster. Our wonderful theorist Giulia Galli has left for a splendid opportunity at the University of Chicago. Dean Lavernia of Engineering and Dean Gibeling of Graduate Studies will leave their positions at the end of their current terms in June 2015 and my current appointment as Interim Dean also ends then. Both the Department of Chemical Engineering and Materials Science and the Division of Mathematical and Physical Sciences (MPS), which currently hosts NEAT, are considering serious structural changes, the outcomes and implications of which are not yet clear. UC Davis is embarking on more aggressive faculty recruitment, with 600 or more hires necessary to meet 2020 growth and replacement of retiring faculty. A number of these recruitments will clearly be in subject areas relevant to NEAT. Plans for a new chemical sciences building are well underway and a committee of faculty, administrators, and facilities people is evaluating current research space and making a long term plan for infrastructure renovations. The Office of Research is seriously studying Organized Research Units and Core Facilities and the manner in which they are chosen, maintained, and reviewed. The Provost is asking for multiyear hiring plans to be submitted through the colleges in Fall 2014. Although NEAT-related HIP (Provost’s Hiring Incentive Program) proposals were not successful, they highlighted the need to work more strongly in areas linking chemistry, physics, and materials science. A blue ribbon committee visited the Physics Department last January to advise on a path forward in experimental condensed matter physics. The new budget model has survived its first year (and so have we). It offers flexibility and opportunities, but also "shimmers" with changes as its unexpected consequences are discovered and, when necessary, remediated.

These streams of change may coalesce into a mighty river, but where will it go and who will thrive in its waters and on its banks? I would like to say that we will thrive; the broad idea of NEAT as "Nano and New Materials in the Environment, Energy, Agriculture, and Technology " (a slightly expanded definition) is as appropriate to Davis now as it was fifteen years ago, but of course opportunities and circumstances keep changing. To chart our future, both intellectually and organizationally, I will be appointing a small faculty advisory committee in the early fall. Its task will be to work with the NEAT community and the departments to reinvigorate NEAT. Clearly at present we are a well tuned grants management organization and we foster individual and small group interactions, but we need to become much stronger, better focused, and do more. It is time for our younger generation to take a more active role. I will help you with enthusiasm but I anticipate stepping aside as director in 1-2 years.

As we all know, the climate for obtaining grant funding is very competitive, and budgets are tight, especially after the end of the stimulus. NEAT has done well; we participate in two renewed (2014—2018) Energy Frontier Research Centers. The Institute for Complex Adaptive Matter (ICAM) continues its activities (with large international participation and funding from member institutions, although the NSF program that funded it for a decade was disestablished, and, under bridge funding, ICAM is seeking other sources of support).

Continuing the reference to flowing water (even in our severe drought, which also is an opportunity for science), it is said that “you never step into the same stream twice”. We must be aware of, and indeed welcoming to, the changing stream. Sometimes we wade, sometimes we swim, sometimes we float, but let us enjoy the journey.
ICAM has held numerous successful workshops and schools in the past year. These include:

- ICAMP 2014, held this past summer in South Africa, the first program we have supported in Africa
- Our first workshop in Austria, with support from the Gordon Moore Foundation, on Quantum Critical Matter

Although ICAM saw the funding from the US NSF International Materials Institute program come to a close as this program was shuttered by the NSF, we were fortunate to receive a bridging award for one year to support ICAM workshops. We also received support from the Gordon and Betty Moore Foundation for workshops on quantum matter. We are moving forward with plans to approach various foundations for support and enter the NSF Partnerships in International Research and Education (PIRE) competition.

The Institute for Complex Adaptive Matter has completed another exciting year of studying emergent phenomena in materials.

The ICAM Annual Conference was held in May in Davis. The Conference began with a rousing channel by UC Davis Chancellor for Research Harris Lewin. We then featured a terrific lineup of distinguished speakers which includes Mike Roukes (California Institute of Technology), Herbert Levine (Rice University), Jing Zhang (Shanxi University), Benjamin Santer (Lawrence Livermore National Laboratory), Craig Fennie (Cornell University), Alessandra Lanzara (UC Berkeley), Sarah Keller (University of Washington). We also heard from recent ICAM Fellows Hassan Masoud, Jennifer Cole, Prashant Jain, Jennifer Misuraca, Luke Somers, Bohdan Senyuk, and Ilya Vekhter.

The night also featured a tribute to ICAM founding director David Pines on the occasion of his 90th birthday. Besides the assembled audience, which featured many friends of David, we had Nobel Laureate Professor Robert Laughlin from Stanford University as a surprise guest, and phone-in tributes from Nobel Laureate (and former postdoctoral associate of D. Pines) Tony Leggett (University of Illinois), Charlie Stichter (University of Illinois), Greg Boebinger (National High Field Magnet Lab), former postdoctoral associate Joerg Schmalian (Karlsruhe), Paul Chaikin (New York University), Argonne National Lab director Peter Littlewood, and ICAM Coordinator Emeritus Rose Romero (Los Alamos National Lab). The evening celebrated David’s career and especially his vision in creating ICAM.

UPDATE: ANSWER PROJECT

The ANSWER (Amyloids for Nanoparticle Synthesis Wiring Energy and Remediation) project made considerable progress in this past year. The group reproducibly made long amyloid fibrils out of genetically re-engineered antifreeze proteins from the spruce budworm insect and ryegrass (see the “backbone cartoons” left), and have preliminary evidence that the spruce budworm protein can not only assemble into long protein wires lengthwise, but also into two dimensional arrays of wires. This is important if these protein building blocks are to be used for synthesizing arrays of nanoparticles for applications to say, photovoltaic.

The group has filed a provisional patent application on their work, and submitted several grant proposals (to the DOE Energy Frontier Research Centers, the DOD Multidisciplinary University Research and Instrumentation Program, and the NSF EFRI2DARE program). While none of these have yet provided support, they have been valuable in building potential collaborations with researchers outside of Davis and in laying the foundations for future funding successes.

The group has “graduated” Dr. Robert Hayre (who founded a Bay Area software startup) and Dr. Hamed Malekan (currently Research Director at ABCO laboratories).
NEAT ORU sponsored a workshop entitled, “Carbides, Nitrides and Related Materials in Earth, Planetary, and Materials Science” held at UC Davis from May 23—24, 2014. This workshop brought together over 60 international scholars from several fields to discuss current trends and future directions in carbides and nitrides research.

Carbides and nitrides, as ceramics, semiconductors, glasses and hard materials, and as possible components in the interior of the Earth and other planets, find increasing attention in geoscience, materials science, and solid state chemistry. The incorporation of small to moderate amounts of carbon and nitrogen into oxygen-containing structures, both as trace to minor substitutions in common oxide and silicates as well as in the formation of new oxycarbide and oxynitride phases, is also a growing field of study and application.

A major focus of the workshop discussion and directions for future research included the nitrogen and carbon components of our and other planets, and in particular, where, under what conditions, and in what forms these elements can be found. A point of discussion was carbon in the form of diamonds, from deep diamonds and nanodiamonds in our own planet, to the possibility of diamonds on exoplanets. For nitrides, discussion revolved around mechanisms for nitride substitution in other minerals, and formation of oxynitrides in the deep mantle.

Major goals of the workshop were to acquaint geoscientists with the work being done in the materials community and to educate the materials community in the fascinating phenomena and problems encountered in our and other planets. Based on workshop discussion, it was determined that materials scientists can contribute to the study of planetary interiors by introducing new analytical techniques to the study of earth materials, and materials created in the lab provide new materials for consideration in natural systems. The carbon and nitrogen reservoir may be a point of interest to draw materials scientists to this research, since the Earth contains such complex combinations of materials interacting in novel and unexpected ways that we are still researching.

Organizers of the Carbide Workshop would like to acknowledge support from the following organizations:

**CARBIDES, NITRIDES AND RELATED MATERIALS IN EARTH, PLANETARY, AND MATERIALS SCIENCE WORKSHOP**

The pressure and/or temperature induced facile transformation of the boron coordination environment in glasses exert important control on their physical properties. Typically, these structural changes are studied ex situ in glasses quenched from their parent liquids subjected to different P-T conditions. Thus, one loses the opportunity of monitoring the mechanism of coordination change in real time or of “seeing” the intermediate or transition state. We have used in situ high-pressure (up to 2 GPa) $^{11}$B solid-state nuclear magnetic resonance spectroscopy in combination with ab initio calculations to investigate the nature of the transition state for the pressure induced BO$_3$® BO$_4$ conversion in a borosilicate glass at ambient temperature [1]. The results indicate that the BO$_3$ planar triangles in the glass structure undergo an anisotropic elastic deformation into a trigonal pyramid that likely serves as a precursor for the subsequent formation of a BO$_4$ tetrahedron (see Fig. 1 at left). Such locally anisotropic deformation of coordination polyhedra under isotropic stress may have far-reaching implications in understanding various stress-induced phenomena in amorphous materials such as stress-induced birefringence and non-Newtonian flow at high strain rates.

RESEARCH HIGHLIGHT: COMPARISON STUDY ON PORE AND MOLECULE SIZE

Determining a reliable mechanism of delivery for nano-sized materials into various systems could be useful for drug delivery, reaction catalysis, CO₂ sequestration, and medical diagnostics. In a recent study published in the Proceedings of the National Academy of Sciences, U.S.A., Dr. Di Wu of the Navrotsky Group and his fellow researchers created a model for nanoparticle delivery which introduced N, N, N-trimethyl-1-adamantammonium iodide (TMAAI) as a guest molecule in a porous silica host. TMAAI was chosen as a representative for other guest organic molecules due to its high melting point causing the material to form a stable near-spherical crystal structure at room temperature (25 °C). The silica host contained pores of various sizes, which allowed the researchers to determine the ideal pore size to carry the TMAAI molecules.

The study identified the importance of the relative size of the guest molecule compared to the pore size in the host material. Pore sizes smaller than 7nm allowed only a single molecule to enter resulting in the greatest confinement effects and were very stable. Intermediate pore sizes between 7 – 12 nm allowed some molecules to enter the pore, but they adsorbed to the surface of the pore, rather than interacting with each other. The largest pore size 12 – 20 nm allowed the most molecules to enter resulting in higher interaction amongst the TMAAI molecules thus forming a stable nanocrystal structure within the pore. This leads to the second important result of these experiments: the microstructure (crystal, amorphous, liquid, etc.) of the guest material in the pores can have a big impact on the stability (or interactions) of the combined guest-host materials. This research provides a foundation for future research into nanoparticle delivery systems in porous frameworks.


RESEARCH HIGHLIGHT: A HIGH PRESSURE NMR PROBE FOR AQUEOUS GEOCHEMISTRY

Professor William H. Casey and his lab members were involved in developing a new instrument for measuring aqueous materials at high pressure. Prof. Casey and his collaborators wanted to be able to measure how elements change species under extreme conditions. They elected to create a modified Nuclear Magnetic Resonance (NMR) probe, which can collect high-resolution molecular data, for samples at high pressure. This new technique will be very beneficial to environmental geochemistry. Researchers will now be able to verify predictions about how processes, such as elemental speciation, petroleum formation, and metal solubility/mobilization, naturally occur in the Earth’s crust.

For a look at this technique in action, check out: blogs.ucdavis.edu/egghead/2014/07/11/reproducing-deep-earth-chemistry/

INTERVIEW WITH GANG-YU LIU AND ALAN HICKLIN ON SPECTRAL IMAGING AT UC DAVIS

As part of his article, “Spectral Imaging/Chemical Sensing: Getting Started with Spectral Imaging”, Mike May interviewed Professor Gang-yu Liu and Alan Hicklin of NEAT’s own Keck Spectral Imaging Facility. Professor Liu addressed the importance of high resolution imaging for use in understanding biological molecules and the importance of genomics. Prof. Liu and Mr. Hicklin developed a process to obtain both molecular information and spectral imaging simultaneously. While this process still needs to be refined, Mr. Hicklin and Prof. Liu are making exciting advances in research capabilities for biochemistry.

For the full article and interview, see:

KEIF Users by Department (2013 - 2014)

- Chemistry 41%
- B&AE 7%
- 15 Other Depts. 8%
- Physics 13%
- E&CE 14%
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- Chem E & MS 1%
- Biochem & Mol Med 4%
- MAE 3%
- BME 3%
- Textiles and Clothing 2%

EQUIPMENT & FACILITIES NEWS

Peter A. Rock Thermochemistry Facility
The 400 W CO2 laser system is in operation. A fast (3 ms) pyrometer was added to the system for recording temperature traces on crystallization. First experiments on drop calorimetry of laser heated levitated samples have been performed.

The third Micromeritics ASAP 2020 instrument was combined with the new Setaram SENSYS Calvet calorimeter for gas adsorption experiments.

Eight commercial and home-built thermal analyzers and calorimeters were upgraded to the Calisto software which provides state-of-the-art acquisition and processing capabilities.

Keck Spectral Imaging Facility
The NanoInk NLP 2000 instrument is an advanced nanolithography device that employs NanoInk DPN technology to create nanoscale patterns on substrate surfaces. The instrument creates such patterns by touching AFM style wicking cantilevers - sharp, ink-coated tips to the surfaces of substrate samples. The NLP 2000 can be used as a nanofabrication platform to create a diverse set of products, such as slides containing nanoscale arrays of capture antibodies that can be used in bioassays.

Training and access to the NLP 2000 can be arranged by contacting Alan Hicklin, the KSIF development engineer.

NEW! Hours of Operation
Monday—Thursday
9 AM—6 PM
Fridays
9 AM—1 PM
2 PM—6 PM

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

First preliminary results from drop-n-catch calorimeter: Y2O3 (L-C transition) ~170 kJ/mol
NEW GRANTS
NEAT ORU RECEIVED AN ESTIMATED TOTAL OF $2.6 MILLION IN EXTRAMURAL FUNDING IN NEAT/ICAM FOR THE CURRENT YEAR.

NEAT PH.D. THESIS

ALEXANDRA NAVROTSKY
- Seyedeh Mahboobeh Hosseini: “Lanthanide Containing Apatites: Synthesis and Calorimetric Studies with Focus on Materials for Solid Oxide Fuel Cells and Drug Delivery” (September 2013)

GANG-YU LIU
- Weifeng Lin: “Characterization of Nanostructures by Near-Field Scanning Optical Microscopy” (July 2013)

WARREN E. PICKETT

FACULTY

Louise Berben received the Organometallics Young Investigator Fellow.

Ricardo Castro is the recipient of the Robert L. Coble Award.

Charles Fadley was awarded an Honorary Doctorate in Physics by the Department of Physics, Uppsala University, Sweden. He also received a Senior Visiting Professorship from the French national program to promote world-class laboratories in physics (Laboratoires d’Excellence: Physique: Atomes, Lumiere, Matiere—PALM).

Kai Liu received fellowship awards from the American Physical Society and the Institute of Nanotechnology (UK), and was elected the General Chair for the 2016 Annual Conference on Magnetism and Magnetic Materials.

Ester Patchin (K. Pinkerton) received the Training Award in the division of Cardiovascular Medicine

Tuan Anh Phan (G. Galli) is the recipient of the prestigious Lawrence Fellowship given by the Lawrence Livermore National

STUDENTS & POSTDOCS

Alejandro Casteneda (K. Pinkerton) received the Interdisciplinary Graduate and Professional Symposium Award.

Dustin Gilbert (K. Liu) received the 1st Prize Margaret Burbidge Award for Best Experimental Research at the 2013 American Physical Society Far West Annual Meeting. He is also the recipient of the by National Research Council Postdoctoral Research Associateship.

Alexander X. Gray (C. Fadley) received the Young Scientist Award, which is an annual award from the User Community of the SPring-8 Synchrotron Radiation Facility in Japan.

Yang Liu (G. Liu) won the graduate student poster award at the Gordon Research Conference for her poster entitled “Signal Transduction by Engineered Extra Cellular Matrices”

Toby Sherbow (L. Berben) received the US Department of Education GAANN fellowship which allows graduate students to focus on their studies and receive mentored teaching experiences.
FRAMEWORK (MOF) HOLDS CO2 TIGHTLY

RESEARCH HIGHLIGHT: METAL ORGANIC FRAMEWORK (MOF) HOLDS CO2 TIGHTLY

The energetics of gases and small and large molecules confined in the internal pores of zeolites, mesoporous silica, metal organic frameworks (MOF) and other porous materials is critical to gas separation, CO2 sequestration, and catalysis. Navrotsky’s group has been developing calorimetric approaches to measure the strength of such adsorption and correlating the thermodynamics with structural and spectroscopic studies. The figure (right) presents one such study, clearly showing several steps of adsorption, corresponding to different adsorption sites, on an environmentally friendly “sugar MOF” which has a strong affinity for carbon dioxide. This is part of expanding collaborative studies on molecular confinement and represents a new direction for the Peter A. Rock Thermochemistry Laboratory.


a) and b) CO2 adsorption isotherms and corresponding calorimetric traces for the first (black) and second (red) CO2 adsorption on the same CD-MOF-2 sample. c) Differential enthalpies of CO2 adsorption for the first (black), second (red) and third (blue) round of adsorption on the same sample.
SUPPORT NEAT ORU

Gifts to NEAT support the diverse, multidisciplinary research and teaching interests of a large number of faculty in many difference academic departments. You may make a gift to NEAT online (giving.ucdavis.edu/ls/NEAT) or fill out and detach the following form with an enclosed check or money order payable to the Regents of California, Davis – NEAT ORU and mail to:

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