

Accelerated B.S./Ph.D. Program

The School of Science offers an accelerated B.S./PhD. program in which students complete the requirements for a Bachelor of Science degree and a Doctor of Philosophy degree in seven years or less from the time they first enter RPI.

Students who have achieved a 3.5 or better grade point average at the end of their first year are invited to apply to the program. After a personal interview, students accepted into the program spend one or two semesters during their sophomore year doing projects in two or three research groups at Rensselaer. Students may choose research groups from any department within the School of Science, based on common research interests with faculty mentors.

Once the students find the right research group, they continue research during the summers and subsequent academic years. Then they make a transition to graduate status at the beginning of, or during, their fourth year of study. Requirements for transition include sufficient credits, maintaining at least a 3.5 GPA, and satisfactory progress in research. The research project, faculty adviser and research group that are chosen as an undergraduate will be the ones in which they continue for their doctorates. While they are undergraduates they receive academic credit during the semesters for their research, and during the summers they receive a stipend.

One of the first two students in the program, Amanda Lund, expects to receive her Ph.D. in May 2009.

Amanda Waite Lund



During Amanda's undergraduate years, she served as co-captain and goalie of the Rensselaer field hockey team, which has repeatedly been recognized as the Division III team with the highest grade point average in the country. Lund was chosen for the association's National Academic Squad during all four seasons of play. She also ranked as one of the best goaltenders in the Liberty League, near the top in categories including save percentage and shutouts.

Amanda's research is being done with George Plopper, Associate Professor of Biology. During her time at RPI she also had the opportunity to participate in coursework at the Lally School of Management and Technology. Their research and teaching efforts focus on the commercialization of new and often disruptive technologies and she was able to apply her learning to issues of biomedical product development and commercialization.

She has accepted a postdoctoral position with Dr. Melody Swartz in the Laboratory of Mechanobiology and Morphogenesis, Institute of Bioengineering at Ecole Polytechnique Federale de Lausanne (EPFL),

Switzerland. She will be moving out there following graduation in July to look at tissue interactions using both in vivo mouse models and complex 3D in vitro culture systems.

At RPI, Amanda's thesis work looks at the use of defined protein microenvironments for the direction and maintenance of stem cell phenotype. Human mesenchymal stem cells are multipotent cells that can differentiate into different tissues within the body including bone, fat, cartilage, muscle and nerve. That differentiation potential I has to be controlled in order to gain access to the full use of hMSC for regenerative therapies. She has focused on the direct interface between human mesenchymal stem cells and a 3D collagen I matrix. Importantly, she is interested in the role dimensionality plays in hMSC differentiation and how that interface can be used to induce and maintain cellular phenotype for bone regenerative therapies. Traditional two dimensional (2D) culture systems create simple models of cell behavior, however, they often lack external mechanical inputs, solute concentration gradients and cell-mediated remodeling of the extracellular matrix (ECM) that are required to form many physiologic structures. The development of cell-based therapeutics is limited by the ability to induce and maintain specific function in vivo. Physiological, three-dimensional (3D) protein hydrogels can be used to create defined cellular microenvironments that provide mechanical and biochemical cues to direct stem cell differentiation while simultaneously allowing for direct cell-mediated reorganization of the naïve matrix. She was able to show that culture of hMSC within 3D collagen I gels provide a more robust bone like response and that this happens in ways that are distinct from 2D culture.

Along this principle, she has also worked on the use of ECM proteins in the induction and maintenance of hMSC phenotype for purposes of regenerative medicine. A novel method of encapsulating hMSC in 3D protein based microspheres (50-150 μ m) was developed, and she was able to demonstrate that these environments could increase the osteogenic potential of hMSC as compared to 2D and agarose controls. She assessed the osteoinductive capabilities of a variety of composite materials and is currently looking to apply this work to an in vivo model of bone formation method of encapsulating hMSC in 3D protein based microspheres (50-150 μ m) was developed able to these environments could increase the osteogenic potential of hMSC as compared to 2D and agarose controls. These microspheres provide a concentrated, local osteoinductive matrix/scaffold that is modular and can be easily manipulated to incorporate critical osteogenic growth factors and matrix proteins to specifically define and maintain hMSC phenotype. In addition, these microspheres can be concentrated into a thick paste that can be minimally invasively injected into a site of injury and fill the whole site of the defect while maintaining void spaces for nutrient diffusion and vascular in-growth.

The Rensselaer Exploratory Center for Cheminformatics Research

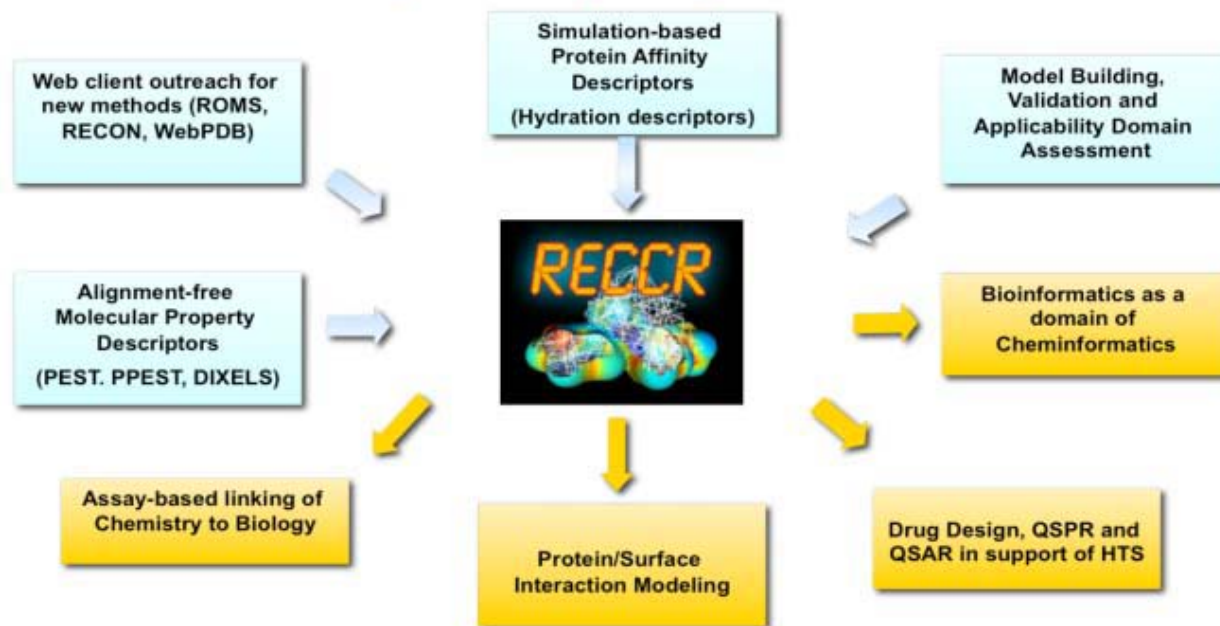
The ability to extract pertinent information from a set of available data is essential in a wide variety of endeavors, as is the availability of tools and expertise to evaluate the validity of the embedded knowledge. This is particularly true in fields where selective interactions between molecules play key roles in establishing material properties, or in modulating biological functions, such as the regulation of metabolic pathways, molecular adhesion in chromatographic systems, control of stem cell differentiation endpoints and the factors that control nanocomposite materials strengths and properties. Databases of assay results for many such properties are either in existence, or are being currently assembled. One of the major challenges in knowledge extraction is that these datasets vary widely in data quality and quantity, requiring the most rigorous data mining and cheminformatics modeling approaches available.

Predictive cheminformatics, as conventionally practiced, often involves a trade-off between obtaining predictive ability vs interpretive ability. Models with good predictive ability are often nonlinear

combinations of descriptors that defy easy interpretation, while simple models constructed from easily interpretable descriptors often do not perform well outside a very limited domain of applicability.

The RECCR Center Vision

Knowledge Discovery Through Cheminformatics



The Rensselaer Exploratory Center for Cheminformatics Research under the leadership of **Professor Curt M. Breneman**, Department of Chemistry, is dedicated to advancing the field of Cheminformatics and increasing the availability of new methods within the Cheminformatics user community. Toward this goal RECCR members are developing new multi-objective machine learning methods, high information-content descriptors, data fusion techniques and infrastructure for extending the reliability and applicability of informatics-based prediction techniques.

The many diverse project areas pursued at RECCR can be grouped into one or more overlapping categories:

Data Generation – using theoretical or experimental methods for creating or extracting knowledge;

Machine Learning and Datamining – model validation, feature selection, pattern recognition, generation of potentials of mean force and knowledge-based potentials;

Property-Prediction – chemically-aware model building, molecular property descriptor generation, Quantitative Structure-Property Relationship modeling, validation, and interpretation;

Applications – utilizing the information made available using the new tools and methods that are developed as part of RECCR.

RECCR emphasizes the central role of Cheminformatics in modern biotechnology efforts, molecular design projects and bioinformatics programs. RECCR will seed new interdisciplinary projects and train graduate students in these areas. The overall goal of RECCR is to continually advance the field of Cheminformatics research and develop descriptors, machine learning methods and infrastructure for extending the reliability and applicability of informatics-based prediction techniques. ADME/Tox predictions, ligand/protein scoring, drug discovery, molecular fingerprint analysis and bioinformatics methodologies would all benefit from advances in Cheminformatics.

Student and faculty research presented at international meeting of the American Geophysical Union

Undergraduate and graduate students from the Dept. of Earth and Environmental Sciences presented their research findings in December at the annual meeting of the American Geophysical Union in San Francisco. The meeting was attended by over 16,000 scientists from around the world. The conference provided the students with a great opportunity to experience the professional side of science, interact with scientists from around the world, and highlight their own research projects at a time when they are applying to graduate schools. We congratulate them on a successful meeting!

Melody Berds, EES Senior

"Fluorine diffusion in titanite: preliminary results from experiments" by M. Berds, J.D. Price, and D. Cherniak

Melody's experiments have yielded new data on fluorine-hydroxyl diffusion in titanite, and her work has important implications for characterizing fluorine behavior in igneous and metamorphic systems. In her research, Melody paired a fluoroapatite source with a low-F titanite, producing diffusion profiles that she analyzed using linear accelerator techniques. The resulting diffusivities showed a limited, albeit scattered, range for the diffusivity of F in titanite for temperatures between 700-900°C. While these diffusivities are notably lower than in other fluorine minerals, F appears to be faster-moving than many other elements within titanite. These data will be important in future research addressing the distribution and retention of F during events associated with tectonism.

Riley Gannon, EES Senior

"Fe-Mg interdiffusion along dry quartz grain boundaries: the dispersed sink method of characterizing grain boundary diffusion" by Gannon, R.S., Thomas, J.B., and Watson, E.B.

Riley characterized diffusion of iron and magnesium along boundaries of mineral grains using a new experimental approach in which the diffusant moves along dry grain boundaries and is incorporated into sink minerals dispersed throughout a polycrystalline rock analog. Riley's experiments showed that the juxtaposition of source and sink materials produced strong chemical potential gradients. The only available pathway for transport from the source to the sink phases was along the grain boundaries. However, the experiments indicate that the grain boundaries become "saturated" in the diffusant, effectively shutting down grain boundary transport; this preliminary result suggests that grain boundary transport may be source concentration dependent. Similar processes may be important in the preservation of diffusive halos surrounding minerals in natural rocks. In addition, his work sheds light on the movement of Fe and Mg, two abundant elements useful in resolving the origin and alteration of many igneous and metamorphic rocks.

Aric Mine, EES Senior

"Tracing the origin of carbonaceous matter and apatite in Neoproterozoic banded iron formations from Abitibi" by A. Mine, D. Papineau, M.L. Fogel, A. Steele, and W. Mueller

Aric did an internship at the Carnegie Inst. in Washington DC last summer, and presented results from the research he did there on ~2.7 billion year old banded iron formations (BIFs) from Québec. Biological oxidation of ferrous iron has been suggested as a possible process by which BIFs form. If correct, organic remains of these microbial communities may be preserved within BIFs. To test this

hypothesis, Aric investigated the organic carbon in the Québec BIFs using Raman spectroscopy, scanning electron microscopy, and stable isotope mass spectrometry. Results indicate that the organic matter was part of the original depositional environment, whereas apatite and carbonate in the BIFs likely formed during diagenesis. Aric found significant carbon isotopic fractionation with large negative carbon isotopic values that consistent with a biological origin of the organic matter, but could not rule out abiological processes as a possibility.

Ben Hallett, EES PhD student

"Retrograde T-t Histories From Pelitic Migmatites Reflect Structural Distance From the Gwillim Creek Shear Zone, Valhalla Complex, British Columbia" by B.W. Hallett and F. S. Spear

Ben's research focuses on the Valhalla metamorphic core complex in southeastern British Columbia, where important evidence of cooling mechanics of metamorphic rocks is recorded in diffusion-zoned garnet crystals. He found core-to-rim zoning of Fe/(Fe+Mg) controlled mainly by diffusion, and modelled the diffusion of these elements in garnet crystals. A difference in the duration of the initial slow cooling steps above a shear zone in the Valhalla complex reflects the time scale of thermal conduction that began when the complex was tectonically thrust onto an effective heat sink. The late cooling history (below 600°C) is poorly constrained by the diffusion profile due to very slow diffusion at these temperatures, but extensive thermochronology is consistent with a period of exhumation by extensional tectonic events.

In addition to the student presenters, EES was well represented at AGU by faculty and post-docs. Interdepartmental research in collaboration with faculty from RPI Computer Sciences was presented by EES Head **Frank Spear**.

Daniele Cherniak and **Jon Price** chaired a session entitled *"Diffusion and Related Transport Processes in Geomaterials"*.

RPI research presented at AGU includes:

Daniele Cherniak

"Ti Diffusion in Pyroxene" by D. J. Cherniak and Y. Liang (Brown)

"Oxidation Dynamics and their Effects on Texture and Magnetic Response in Remelted and Quenched Submarine Basaltic Glass" by K. Burgess (Brown), R. F. Cooper (Brown), D.J. Cherniak, J.A. Bowles (Minnesota), J.S. Gee (Scripps UCSD)

Rob McCaffrey

"Vertical axis rotations observed in geodetic and paleomagnetic data" by R. McCaffrey - invited

"Inverting geodetic time series for secular and transient deformation sources: Application to slow-slip at subduction zones" by R. McCaffrey - invited

"Recurring slow slip on the Hikurangi subduction interface, New Zealand" by J. Beavan (New Zealand GNS), L. Wallace (New Zealand GNS), and R. McCaffrey

"Geodetic Observations of an Earthquake Cycle at the Sumatra Subduction Zone: The Role of Interseismic Strain Segmentation" L. Prawirodirdjo (Scripps), Y. Bock (Scripps), R. McCaffrey, C. Subarya (Indonesia National Survey), P. Fang (Scripps)

Jon Price

"REE Diffusion on Quartzite Grain Boundaries: Preliminary Results from Experiments" by J.D. Price and E.B. Watson

Frank Spear

"MetPetDB: New Directions for Metamorphic Studies" by F.S. Spear, S. Adali (RPI Computer Sci), B.K. Szymanski (RPI Computer Sci), B.W. Hallett, A.J. Waters (RPI Computer Sci), Z.J. Linder (RPI Computer Sci), M.E. Fyffe (RPI Computer Sci), D. Goldfarb (RPI Computer Sci), and K. Barlett (RPI Computer Sci).

Jay Thomas

"Titanium Under Pressure: Assessing the Effect of Pressure on the Ti-in-Quartz Geothermometer" by J.B. Thomas and E.B. Watson

Bruce Watson

"The Effect of Growth Kinetics on the Development of Element- and Isotope Profiles in Single Mineral Grains" by E.B. Watson and T. Mueller (Ruhr-Universität Bochum) - invited

"Preliminary Results on Fractionation of H, C, S and Cl Isotopes by Thermal Diffusion in Silicate Melts" by E.B. Watson, N. Shimizu (WHOI), R.L. Hervig (Arizona)

Anahita Tikku

Also representing EES was former Research Associate Anahita Tikku (now at ExxonMobil) presenting research completed with Steve Roeker during her time at RPI:

"Continuous gravity measurements from Kilauea Volcano Hawaii'i, 2007-2008" by A.A. Tikku, M. Poland (USGS -HVO), S. Roeker, and P. Okubo (USGS-HVO).

The Center for Initiatives in Pre-College Education (CIPCE)

Lester Rubinfeld, Director

- The Center received a \$118,750 grant from the New York State Department of Education under its "Teacher Quality Leadership Program (TLQP)" to work with local K-8 teachers. Rubinfeld, and Josephine Carnevale Seddon, CIPCE's Project Manager for Teacher Professional Development, are working with teachers in six local schools: two K-5 schools in the Cohoes School District; two K-6 schools in the Troy School District; and two K-6 Charter Schools in the Albany area. The work, which focuses on mathematics teaching, seeks to address several objectives. One is to deepen teachers pedagogical skills by working with them on inquiry-based activities. A second is to work with teachers to recognize the gaps in the mathematical understanding of their students, and how to overcome them. And the third is to expose teachers to educationally sound interactive media, and how to integrate these materials into classroom mathematics teaching.

- The Center is presently conducting after school, LEGO Mindstorm Robotics activities with inner city youngsters in five local schools (North Albany Academy and Meyers Middle Schools in Albany; Rensselaer Middle School; School 12 in Troy; and the Green Tech High School in Albany), and two neighborhood-based youth organizations (the Trinity Institution in Albany and the Troy Boys and Girls Club). These activities are coordinated by Melissa Hershey, CIPCE's Project Manager for Technology and Engineering Activities. A group of twenty Rensselaer undergraduates, from a wide variety of majors, are trained by CIPCE and co-facilitate these activities. The objective is to expose young people to the wonders of constructing and

programming robotics objects, with attached sensors, so that they can behave intelligently and react to their environments.

- The Center recently received a \$20,000 grant from the Intel Corporation to sponsor a Local FIRST LEGO League competition. In addition, Intel provided \$500 awards to eight teams to offset the costs of preparing for the competition, which was held on Rensselaer's campus on Saturday, December 6. The competition was coordinated by Melissa Hershey, CIPCE's Project Manager for Technology and Engineering Activities, and Michele Murray, CIPCE's Administrative Coordinator. A total of twenty four teams from all over the Capital District competed against each other to address a series of eighteen engineering "missions" focused on the earth's climate. Ten awards were given out in the areas of Robot Design, Robot Performance, Robot Consistency and Team Spirit. There were over sixty people volunteering many hours of their time, who made this competition a class act.

Faculty News and Notes

Promotions effective July 1, 2009

Petros Drineas – Computer Science - to Associate Professor with Tenure

Professor Drineas' research interests lie in the design and analysis of randomized algorithms for common matrix operations and decompositions (e.g., matrix multiplication, SVD, etc.). This work spans the Theoretical Computer Science and the Numerical Linear Algebra communities, as well as the Data Mining and Information Retrieval communities. Particular emphasis has been placed on the design of provably accurate and computationally efficient algorithms. Along with his students and collaborators, Prof. Drineas has worked on applying such algorithms to data mining tasks in three application domains: the analysis of human genetics data (medicine and biology), the analysis of data from testing the functionality of electronic circuits (electrical engineering), and the analysis of collaborative filtering and document-term data (internet). A large number publications in leading journals and conferences indicate that the proposed methods have significant impact in data analysis.

Bulent Yener – Computer Science – to Professor

My Professor Yener's recent interest is on both systems and theoretical research in the area of complex systems that include data, communication, and biological networks. He currently pursues two research tracks (i) modeling, analysis, and prediction of time evolving biological systems (such as stem cell differentiation, tissue repair process, epileptic seizure onset); and (ii) routing and control (such as synchronization and scheduling) and security problems (such as key extraction and authentication algorithms) in wireless ad hoc networks. The funding for the first research area is obtained from NIH R01 grants. The second area is funded by NSF and AFRL grants.

Mohammed J. Zaki – Computer Science – to Professor

The overarching theme of Prof. Zaki's research has been on developing novel, efficient, and scalable data mining techniques for massive datasets, with special emphasis on applications in bioinformatics. He is particularly interested in mining patterns and motifs in diverse datasets ranging from genomes and proteins, to complex graphs and networks. He is also interested in scalable indexing methods for these problems.

Other News of Faculty

Sang-Kee Eah

Matthew Martin, a graduate student in the Department of Physics, Applied Physics, and Astronomy made his first presentation at 2008 Materials Research Society Fall Meeting at Boston. The poster was titled, "Monolayer Film of Gold Nanoparticles on a 3 inch or Larger Silicon Wafer" by Matthew N. Martin and Sang-Kee Eah (Assistant Professor of Physics). He had only one 5-second break during the 3.5-hour poster night due to so many questions, and received an invitation to apply for a National Research Council postdoctoral fellowship at the National Institute of Standards and Technology. By invitation for future collaboration he visited a professor at Harvard University, where he attended the 37th New England Complex Fluids (NECF) Workshop. The 43rd NECF workshop will be hosted at RPI in June, 2010 by Patrick Underhill (Assistant Professor of Chemical Engineering) and Sang-Kee Eah.

Joel Giedt

Assistant Prof. Physics, together with collaborators, submitted "Lattice super-Yang-Mills using domain wall fermions in the chiral limit," to Physical Review D, preprint <http://arxiv.org/abs/0810.5746>.

This article is the culmination of research into the gaugino condensate in super-Yang-Mills, utilizing the CCNI. It was found that the condensate is nonzero, a necessary ingredient for most phenomenological models of spontaneous supersymmetry breaking. In total the project required 30 million BlueGene/L core hours, and is the most extensive simulation to date of a supersymmetric lattice gauge theory.

Prof. Giedt presented these results at "Dynamical Electroweak Symmetry Breaking," Sept. 9-13, Odense, Denmark.

Michael Shur

Patricia W. and C. Sheldon Roberts Professor of ECSE and Physics, had a letter on bio testing by N. Pala and Michael Shur chosen by Electronics Letters as Letter of the Month, <http://www.ietdl.org/EL>.

Ingrid Wilke

Associate Professor of Physics visited Union College in Schenectady and the University of Massachusetts Amherst giving presentations on "New Developments in Terahertz Spectroscopy" in the Chemistry Seminar at Union College and on "Terahertz Spectroscopy and Imaging" in the Condensed Matter Seminar at UMass Amherst.

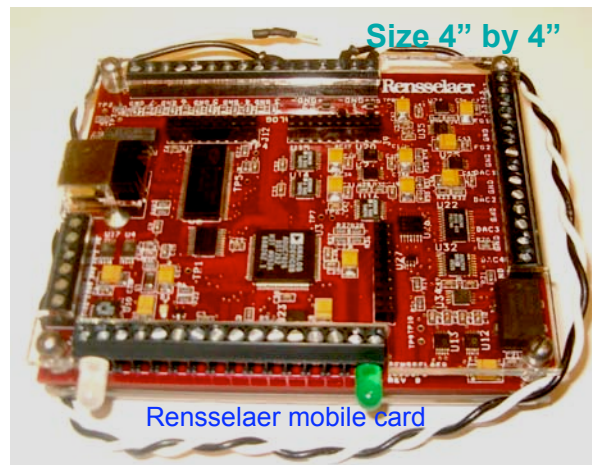
Jeff Trinkle

Professor of Computer Science, was an invited speaker and panelist for the National Science Foundation's information session on Cyber-Physical Systems, a new \$33M program. Cyber-physical systems are physical systems characterized by embedded distributed computation, communications, actuation, and sensing, such as smart homes, robots, and ocean-monitoring systems.

Jeff Trinkle is the general chair of the annual international conference, Robotics: Systems and Science (<http://www.roboticsconference.org/>), to be held in Seattle WA, in June 2009.

Peter Persans

Professor of Physics, used the Rensselaer Mobile Studio IOBoard (www.mobilestudio.rpi.edu) and associated software in an introductory electromagnetism and waves course.



The IOBoard connects to the user's PC via USB, providing an inexpensive multipurpose instrument with functional capabilities of oscilloscope, audio output, and function generator. This project entitled, "Hands on physics outside the classroom", is funded by the NSF as a joint collaboration between the Physics (Wang, Persans, Ciolek, and Dwyer) and ECSE (Millard) departments. Students can perform physics experiments anytime, anywhere.

During fall 2008, students in a test section used the IOBoard to extend experimental activities outside of the classroom. For example, in one activity they explored the properties of an RC circuit as an ac voltage divider in class and the properties of an RL circuit outside of class on their own. A preliminary analysis of student performance on test questions showed a mastery of associated topics at a level higher than those students who did not take advantage of the hands-on IOBoard outside the classroom.

** This newsletter is prepared monthly and distributed to School of Science faculty, staff, students and alumni to highlight accomplishments and events within the school. Please submit news items for the next newsletter to Samuel Wait, Associate Dean of Science, at waitsc@rpi.edu.*