

RESEARCH SPOTLIGHTS



Fourth-year student **LAUREN BAETSEN** and second-year student **ANTHONY SUNG**, both from the biomedical engineering department, are part of an international community using 3D printing to develop a new class of open source, affordable prosthetics. Their work, under the supervision of Professor David Chen, contributes to E-nabling the Future, a group of more than 1,500 international members that collaborate to create and print 3D assistive hand devices for those in need. The effort is also part of a U.Va.-Coulter Translational Research Partnership initiative to promote greater cross-disciplinary utilization of 3D printing and explore the potential of applying this technology to prosthetic design. The students' partnership came together last year; Baetsen started working on the project after taking Professor Chen's Advanced Design class because the research allows her to pursue her passion of developing new prosthetics and orthopedics, and Sung joined her after gaining experience with Computer Aided Design (CAD) software while conducting research with Professor Chen last spring. Together they are using CAD and

open source tools to demonstrate the potential of this revolutionary technology.

Since starting work on the project last spring, the team has collaborated with the mechanical engineering Rapid Prototyping Lab to create a functional prosthetic hand. Using the open source Web site Handomatic Baetsen and Sung size a generic hand design to fit its new owner. They enter measurements of different portions of a hand and select the desired features to produce a 3D-printable file that can be quickly assembled in lab for a new owner. This fast production time is just one advantage of 3D printed prosthetics.

Although 3D printed prosthetics are not yet capable of matching high-end prosthetics in fine motor skills and sensory applications, the pair's model will help the user complete gross motor tasks, such as picking up objects or gripping the handlebars on a bike, which can greatly improve quality of life. The prosthetic is also different from more traditional devices because it utilizes tension wires instead of electronics to generate grip strength for fully mechanical operation, saving energy. The low production cost of about \$50 is yet another benefit, as comparable electronic devices can cost thousands. A further advantage of this class of prosthetics results from a developing 3D printing collaborative network. Files can be shared and used by anyone with a 3D printer of sufficient quality to manufacture the prosthetic. New designs can be uploaded to open source databases, where high-quality prosthetics can be created, shared and iterated by students and 3D printing enthusiasts across the world—allowing design improvements to be made rapidly at low cost by anyone with sufficient technical skills.

Baetsen and Sung are currently working to improve the tolerances of their design, so that it can be manufactured by lower-precision 3D printers. They hope to design their own more user-friendly artificial hands in the future by adding more technical capabilities and improving the model's appearance. Their project demonstrates the potential of 3D printing resources available to students at U.Va. and they hope their work will inspire further undergraduate 3D printing projects and lead to greater interdepartmental collaboration in 3D printing.



AYODEJI BODE-OKE is a fourth-year aerospace engineering major currently working with Professor Haibo Dong and graduate student Samane Zeyghami, to study the effect of wing shape change on the kinematics of dragonflies. Professor Dong inspired Bode-Oke to start his research during a thermodynamics class two years ago.

Recent advancements in high-speed photography and photogrammetry have enabled most of the advances in insect flight dynamics and aerodynamics research. However, wing shape change or wing damage is not thoroughly understood, and most of the current research only gives a biological approach to the problem, as opposed to Bode-Oke's team's engineering approach. Ayodeji's work aims to determine what happens to flight behavior when the wing of a dragonfly is damaged in order to understand what happens when the wing of a flapping microaerial vehicle is damaged.

Using high-speed video cameras and 3D surface-reconstruction software, he has obtained details about the motion, and is currently analyzing results. Thus far, Bode-Oke has recorded videos of dragonfly flight and reconstructed them using the software Maya. He has finished processing the wing and body kinematics and drawn conclusions suggesting that chordwise damage is more detrimental than spanwise damage. He notes that when insects damage their wings, they do not lose their turning ability. They can still perform the same maneuvers as when their wings were intact, although it takes a longer time to perform the maneuver. In addition, based on the kinematic analysis, spanwise damage is more efficient, which could explain why insects have evolved, as spanwise damage occurs more frequently.

So far, wing damage is only one of the problems Bode-Oke has been able to tackle. In his research, Bode-Oke hopes to establish a new view of the effect of damage on flight. His team's findings contradict the general assumption that when wings are damaged because of loss in area, the other wings have to compensate, flapping faster with higher stroke amplitude. He hopes to establish this work as the first to have engineering significance, whereas others have focused on biological significance such as forage behavior, which is how damage affects feeding abilities. His group's findings have far-reaching consequences for MAV wing design, wing kinematics control design and a number of other areas.

The manuscript for Bode-Oke's research is under preparation and will be submitted in the first quarter of 2015 to either the Journal of the Royal Society Interface or the Journal of Experimental Biology. Zeyghami presented the team's preliminary results at the American Physical Society Division of Fluid Dynamics conference in November 2014. Bode-Oke hopes to continue this research if he remains at U.Va. for graduate school and will likely focus on biology-inspired engineering research.



TAEHUN KIM, a fourth-year student in chemical engineering, works with batteries, researching ways to modify these energy storage systems to make them more efficient at harnessing and utilizing energy. Kim's work focuses on investigating ways to improve rechargeable lithium ion batteries (LIBs) through his research with Professor Gary Koenig in the chemical engineering department. Since beginning research in the spring of 2014, he has studied the cathode materials used in lithium ion electrochemical cells and optimizing overall performance of the batteries.

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Kim received funding from the nanoSTAR Institute at U.Va. and hopes his research will improve the design of LIBs to commercialize their use in electric vehicles, thus addressing increasing energy demands and lowering greenhouse gas emissions.

LIBs efficiently store energy in a chemical form, offering very high energy density compared with other common batteries, such as lead acid or nickel metal hydride. Due to these characteristics, this battery is a good candidate to be an advanced power source for electric vehicles. The cathode active material in LIBs represents about half the cost of the main materials used in LIB; thus, reducing the cost of the cathode active material would make LIBs more widely available. While these batteries are commonly found in consumer electronics such as cell phones and laptops, this technology is not yet able to be fully commercialized with applications, such as electric vehicles, that consume energy and drain power at higher rates. Improvements to current LIBs are necessary for electric vehicles to become commercially viable.

Kim's research aims to increase the energy density and rate capability of the batteries to increase storage and power output to meet the energy demand required to turn motors. He carried out LIB cathode active research, changing physical properties and material characteristics of the precursor materials for the cathode active materials and observing the effectiveness of such changes. By tuning properties of the precursor materials such as size, structure, composition and morphology of the particles, Kim can increase the charge capacity of the LIB and optimize the design. He observed the synthesis of various precursors and reported the optimum method to create such particles.

Kim will present his research at the nanoSTAR spring symposium in 2015. He is passionate about the possibilities LIBs hold for the future of electric vehicles and sustainable energy storage and conversion. He is eager to continue his research with lithium ion battery cathode active materials and see what the future holds for LIBs. He plans to further his chemical engineering education in graduate school and hopes to continue studying in the energy storage and conversion field.



ZEMING LIN is a third-year student studying computer science. As a firm believer in using computers to automate as many tasks as possible, he is fascinated by deep learning, particularly its hands-off nature. Deep learning is a set of algorithms in machine learning, a discipline that examines the construction and study of algorithms that can learn and adapt from data. The science is based on representation learning, which converts raw data input into a representation that facilitates analysis. A particularly unique feature of deep learning is that it is fast and scalable, unlike most machine learning algorithms. In an increasingly data-driven world, deep learning holds a lot of potential for processing massive volumes of data, making it applicable to various fields, such as content serving and computational biology.

Lin works in Professor Yanjun (Jane) Qi's lab, where the research focus is on machine learning and bioinformatics. His research explores the applications of deep learning to bioinformatics. With a series of 28 tasks, he seeks to predict proteins' functional properties using deep neural networks, which are statistical learning algorithms inspired by their biological counterpart. Due to their adaptive nature, deep neural networks are commonly used to estimate functions that can depend on many inputs. In Lin's research, deep neural networks are used to build a model that can

predict an output, like a protein local property, from a given input, like a portion of a protein sequence.

Each of the tasks in his research project has a number of labels, which are the local properties of the protein, predetermined from prior studies. The tasks include predicting proteins' solvent accessibility, transmembrane topology, two secondary structure alphabets and identifying structural elements like DNA-binding residues, protein-binding residues, signal peptides and coiled-coil regions. Their project aims to build a model using known successful neural network techniques to create a survey of how well these techniques run on a protein sequence data set. They also hope to train their model on all tasks at the same time. This "multitask" approach allows the model to use the commonality among the tasks to achieve better results.

Using deep learning techniques, Lin and Professor Qi hope to create a comprehensive study and to release their dataset to pioneer more research into the applications of deep learning to computational biology. Deep learning has been applied heavily to other fields such as image search and facial detection, but not to computational biology, although there seems to be much potential in that field. They look to submit their work to the *Journal of Machine Learning Research*, the International Conference on Machine Learning and potentially other bioinformatics-related conferences.



ANNE MENEFEE hails from Richmond, Virginia and is a civil and environmental engineer in her fourth year. An avid environmentalist, Menefee is interested in both sustainable energy and climate change mitigation.

Since sustainable energy and climate change have been highly politicized, she feels that the current actions taken to address them are insufficient, given their urgency. Thus, the main driving force of her research is to develop tangible solutions to these pressing issues.

Under the mentorship of Professor Colosi Peterson, Menefee has been researching the sustainability of algae-based biofuels in a team with fourth-year students Shelley Parekh, Jessica Murray and Kwasi Twum-Acheampong, and graduate student Shanshan Peng. With increasing concerns over climate change and energy security, paired with substantial political pressure, the drive for alternative energy sources has increased in recent years. Menefee's research focuses on algae-derived biofuels, a potential new generation of biofuels that seem to be a promising alternative to current biofuels because they do not compete with food crops or arable land. Additionally, algae are energy rich and are able to grow year-round in nonideal environments, furthering their promise. However, the intense nutrient demands of algae impede their large-scale feasibility, leading to interest in integrating nutrient recycling with production processes. Current understanding suggests that nutrient recycling is compatible with hydrothermal liquefaction (HTL), a promising algae biofuel production pathway. Nevertheless, efforts to commercialize these systems have shown lower biomass yields in algae cultivated using the recycled aqueous co-product (ACP) streams from HTL, when compared with using standard media, such as a nutrient source. With her team, Menefee aims to identify factors leading to this growth inhibition in algae cultivated through ACP as opposed to standard media. By identifying these factors, appropriate modifications can be made to these systems, ultimately allowing algae to become a viable and sustainable large-scale biofuel feedstock.

Last fall, Menefee and her team researched the effects of pH and phenol on algae growth, as literature indicated significant differences in these factors between the composition of ACP streams and standard growth media. They found that pH alone is not a driving cause of reduced biomass yields, but phenol has a significant inhibitory effect on algae growth at a concentration and pH levels characteristic of ACP streams. Phenol's inhibitory effects were observed after a retention time

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of 10 days, the length of time algae is cultivated before processing in the commercial-scale algae biofuel production systems they are studying. Since phenol's inhibitory effects were observed after the retention time in the production systems of interest, this result is particularly relevant to their objectives.

With their research, this team has earned first place in the "Outstanding Presentation" category at the 2014 Civil Engineering Research and Design Symposium, a culmination of the all the Capstone projects in the civil and environmental engineering department. They also hope to submit their research to the Undergraduate Research and Design Symposium this spring. Menefee will continue working on this research project with Shanshan Peng, the graduate student on her team, through the end of this school year. Next year, Menefee hopes to pursue environmental engineering in graduate school, with a focus on applications of environmental chemistry to the energy sector.



ALEX YANG is a third-year chemical engineering and economics double major with a computer science minor drawn to Professor Michael Shirts' computational approach to chemical engineering, Yang decided to conduct research under this professor during his second year. Since then, he has been actively involved in researching the protein lacritin and its interactions with the eye's tear duct system. His research has implications for dry eye, a condition affecting nearly 5 million Americans, and explores potential applications of the protein to address this issue.

Working with Professor Shirts, Yang researches how the lacritin protein works to increase basal tearing. It is very impractical and costly to embed lacritin within a drug and mass produce it, which is why he is working to develop a smaller molecular analog yielding similar results. Using such an analog is advantageous because the smaller molecule would retain just the functional portion of the protein.

Yang uses molecular simulation techniques to analyze the interactions of lacritin at the atomic level. Through this method of study, he can identify functional sites and witness how mutations within peptides change the behavior and dynamics of the molecules without the expensive and time-consuming experimental laboratory techniques. While much work remains to be done, Yang has been using conformational analysis and simulations to understand the structure of the compound, the active sites where the protein receptor will bond and which amino acids will stabilize the active sites. He has been comparing how the secondary structure of the lacritin changes upon rotation when compared to that of the smaller molecules, because if the two have similar structure, their behavior should imitate each other. To make this analysis, Yang writes code to compute and observe trends in the radius of gyration, which is the distribution of atoms around an axis of rotation. By understanding how the protein is shaped and reacts with its receptor, syndecan-1, Yang's work will allow others to design molecules to mimic this mechanism to create a more effective treatment for dry eye.

Yang enjoys challenging himself by utilizing his knowledge from class and applying it to new fields. He has enjoyed studying the combination of computational and quantum chemistry through a previous internship and wished to continue learning about new depths of the chemical field, especially the developing field of protein dynamics. Working with Professor Shirts and faculty at James Madison University and Fort Belvoir, Yang has given presentations and reports discussing the future steps for this study. He has also presented during the 2014 American Institute of Chemical Engineers Annual Student Conference and hopes to publish the results of his research in the near future.