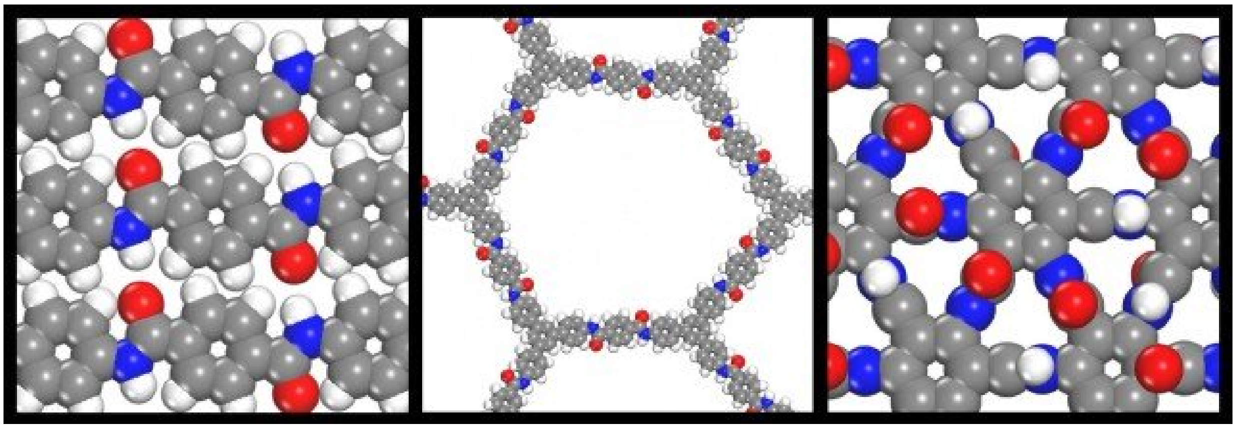
Collaboration leads to 2-D polymer discovery

February 25 2021



Credit: The Army Research Laboratory

Army researchers reached a breakthrough in the nascent science of two-dimensional polymers thanks to a collaborative program that enlists the help of lead scientists and engineers across academia known as joint faculty appointments.

Researchers from the U.S. Army Combat Capabilities Development Command, now known as DEVCOM, Army Research Laboratory partnered with Prof. Steve Lustig, a joint faculty appointment at Northeastern University, to accelerate the development of 2-D polymers for military applications.

The collaboration with ARL Northeast led to a groundbreaking study published in the peer-reviewed scientific journal *Macromolecules*. Editors featured the research in a cover article.

"2-D polymers have been studied very seriously from a synthetic viewpoint for only about 10 years," said Dr. Eric Wetzel, research area leader for Soldier Materials at the laboratory. "They represent a new, relatively unexplored class of materials with tremendous potential."

According to Wetzel, 2-D polymers have a very repeatable, symmetric pattern akin to "chicken wire," which offers access to more structural enhancements compared to one-dimensional, linear polymers like Kevlar.

In an effort to gauge the full potential of these materials, Army researchers have started to computationally design 2-D polymers in the hopes that they may develop a superior alternative to conventional aramid fibers for applications such as armor and fire-resistant clothing.

Prof. Steve Lustig, a joint faculty appointment at Northeastern University, uses his industry experience with DuPont to help Army researchers calculate the environmental durability of simulated 2-D polymers.

In order to properly create a 2-D polymer that can withstand real-world conditions, Army researchers sought the aid of Lustig, who previously worked at DuPont Central Research & Development for over two decades before he became an associate professor with tenure at Northeastern University.

"The idea of the 2-D polymer project is essentially to make a 2-D version of Kevlar," Lustig said. "I had over a decade of experience working with the Kevlar business in various aspects of liquid crystalline polymer polymerization, processing and properties. The ARL team believed that my background would be helpful."

Lustig explained that he had first learned about the laboratory in the mid-2000s when he came in contact with Dr. Kenneth Strawhecker, an Army scientist who had reached out to DuPont in search for industry collaborations.

At the time, Lustig worked as a lead scientist in DuPont's polymer physics group and specialized in the development of novel tools for statistical mechanics, statistical thermodynamics and molecular simulations.

In addition to his expertise on the computational side of industrial research, he also conducted experiments in chemical synthesis, polymer processing, polymer material property characterization and atomic force microscopy.

"I have never had the patience to stay in one place and become a master in just one very small area," Lustig said. "I've always tried to solve problems holistically using experiments, theory and computers."

Once Lustig met with Strawhecker, the two began a series of informal collaborations that focused on the use of atomic force microscopy to understand not only the structure of Kevlar materials but also their response to tensile strain and bending mechanics.

The scientific journal *Macromolecules* features the Army-led study on the inside cover of its latest issue.

The American Chemical Society later published the outcome of this research as the cover of the peer-reviewed scientific journal *Applied Materials & Interfaces* in 2020.

Even after Lustig left DuPont in 2016, he continued his collaborations with the laboratory as a visiting scientist. Shortly after one of his seminar presentations at the lab, he met Wetzel, who immediately recognized the value of Lustig's industry experience.

Over the course of his continued interaction with Strawhecker and Wetzel, Lustig obtained the opportunity to become an ARL Joint Faculty Appointment after he joined the Department of Chemical Engineering at Northeastern University.

Due to his close proximity to ARL's Northeast campus, both Strawhecker and Wetzel saw Lustig as a top candidate for the position.

"The ARL Open Campus Initiative provides a way to tap into outside expertise that may not exist within our laboratory," Wetzel said. "The joint faculty appointment is a new construct within Open Campus that has only existed for a few years, but we were able to integrate an expert with years of experience at DuPont into our research program thanks to this mechanism."

According to Wetzel, Lustig's long history with high performance fiber development projects at DuPont provided Army researchers with access to unique modeling capabilities as well as invaluable guidance on the methods and techniques that would enhance the stability of their conceptual 2-D polymers.

As a joint faculty appointment, Lustig analyzed the environmental durability of the lab's 2-D polymer designs and ran computer simulations that determined how well they endure extreme conditions such as intense heat.

Lustig worked alongside Dr. Jan Andzelm, an Army scientist and ARL fellow whose expertise in the molecular simulations of polymers were critical for running the calculations.

Through these computer simulations, the researchers compared the thermal stability of the 1D polymer Kevlar, a 2-D polymer called an amide covalent organic framework, known as amCOF, and a hypothetical 2-D polymer designed by the laboratory called graphamid.

"We performed a series of very accurate, high-level quantum mechanical calculations called ab initio molecular dynamics and studied the changes in the structure between the three molecules we looked at," Lustig said. "Once we confirmed that our method could accurately describe a well-known molecule like Kevlar, we could apply it to molecules we didn't know like graphamid and make accurate predictions about their behavior and properties."

The results of the comparison study showed that graphamid could potentially withstand temperatures as high as 700 degrees Celsius, which exceeded the limits of both Kevlar and the amCOF material.

Given the study's acceptance as a cover article, Lustig said he believes that the team's latest success clearly highlights the importance of ARL Open Campus initiatives such as the joint faculty appointments.

Lustig expressed his gratitude to the laboratory for his position and mentioned how he viewed the opportunity as an excellent way for him to help the Army with its efforts.

"I got involved with Kevlar in the first place because my father was career Army, so the idea of protecting guys like my dad is really important to me." Lustig said. "I feel very excited that we'll be able to offer Soldiers new materials to make their work easier and safer."

More information: Steve R. Lustig et al, Highly Thermostable

Dynamic Structures of Polyaramid Two-Dimensional Polymers, *Macromolecules* (2020). DOI: 10.1021/acs.macromol.0c01931

Provided by The Army Research Laboratory