Developing a model critical in creating better devices

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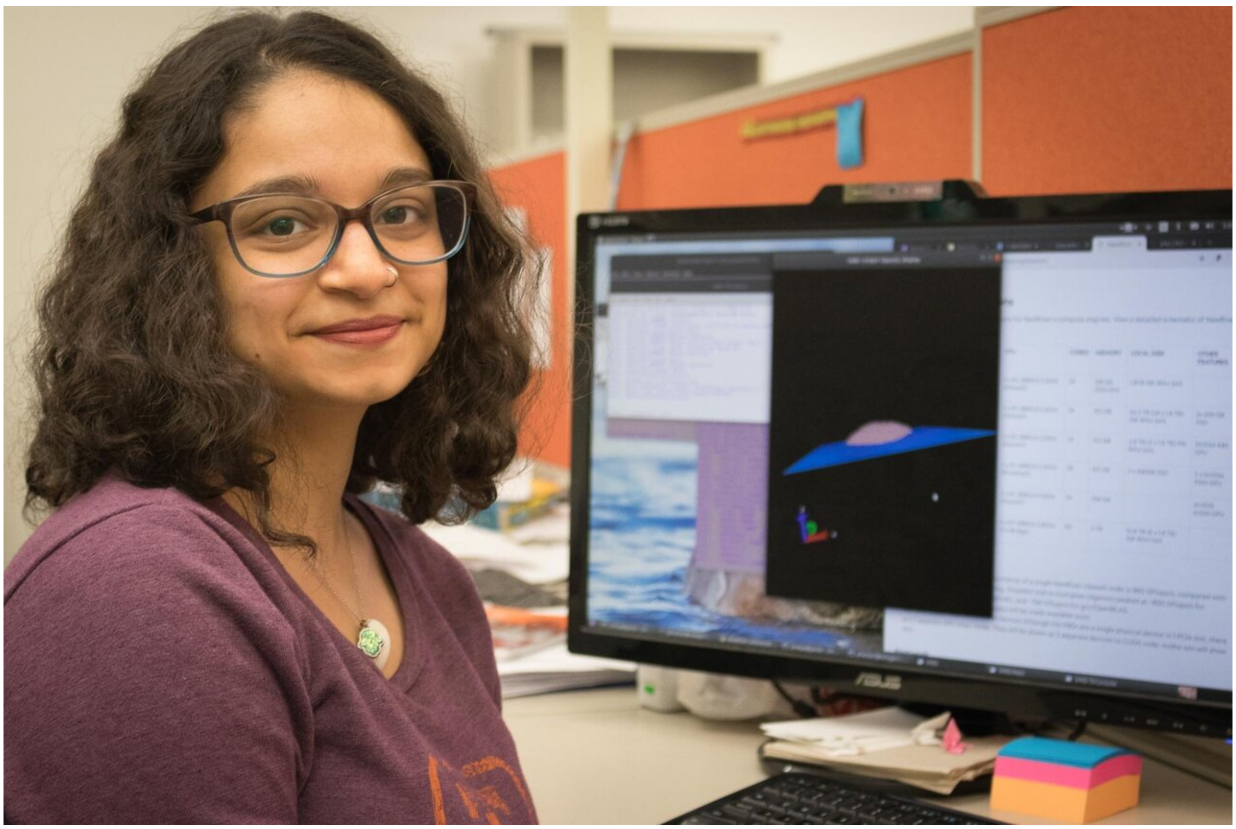

Chemical engineering junior Preeya Achari Credit: Virginia Tech

Water is everywhere. Understanding how it behaves at an intersection with another material and how it affects the performance of that material is helpful when trying to develop better products and devices.

An undergraduate researcher at Virginia Tech is leading the way.

Chemical engineering junior Preeya Achari has now developed and recently published as first author a new computational model to better understand the relationship between water and a type of two-dimensional material that is composed of one-atom-thick layers that are flat like a sheet of paper.

The model will help predict the behavior of water at the surface of hexagonal boron nitride, a compound commonly used in cosmetic products, such as eyeshadow and lipstick.

The compound is similar to graphene, which has already shown great potential in lubrication, electronic devices, sensors, separation membranes, and as an additive for cosmetic products. Hexagonal boron nitride, however, has a few more favorable properties, such as its higher resistance to oxidation, flexibility, and greater strength-to-weight ratio—properties that could also be useful in the production of nanotechnology, drug delivery, and harvesting electricity from sea water.

Prior to the development of the new model, understanding the molecular-level structure of water at the contact surface with hexagonal boron nitride proved very challenging, if not impossible. The development may provide more control in performance of devices made with hexagonal boron nitride and water.

"This knowledge can help in improving the performance of boron nitride-based electronic devices," Achari said.

Achari works in the computational lab of chemical engineering assistant professor Sanket Deshmukh. She developed the model in close collaboration with others in Deshmukh's lab, including post-doctoral researcher Karteek Bejagam and visiting scholar Samrendra Singh.

Achari arrived at Virginia Tech looking for a challenge and was drawn to working with the unfamiliar field of computational materials science—a field that utilizes computational methods and supercomputers to understand existing materials and accelerate materials discovery and development. She found Deshmukh's lab during her sophomore year and has balanced her time as an undergraduate researcher and a full-time student ever since.

"It is extremely satisfying to see the results of my lab's hard work and to look back at everything I contributed and learned along the way," Achari said. "I also value knowing that the work that my lab and I do will go on to benefit other researchers in my field."

In addition to her recently published journal article, Achari was also awarded best oral presentation at the 2018 Materials Research Society meeting in Boston, Massachusetts.

More information: Preeya F. Achari et al, Development of non-bonded interaction parameters between hexagonal boron-nitride and water, *Computational Materials Science* (2019). DOI: 10.1016/j.commatsci.2019.02.011

Provided by Virginia Tech

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