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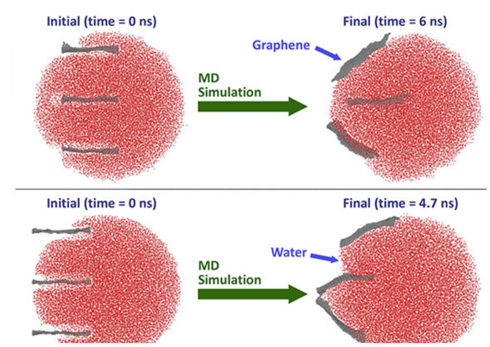
SDSC's Comet Supercomputer Used to Model Graphene-Water Interaction

Study suggests graphene may assist in administering drug delivery

Graphene is a two-dimensional material with a single atomic layer of carbon that has a hexagonal structure, similar to a honeycomb. A single layer of graphene, which is more commonly known as a single layer of graphite, such as pencil lead, is 97 percent transparent, stronger than steel, almost weightless, and can conduct electricity.



One layer of graphene is so thin that it takes a million layers to make it one millimeter thick. A simulation done using SDSC's Comet supercomputer shows a cross-sectional view of seven graphene flakes in a water droplet, and that the multi-layered graphene eventually merges together. Credit: Solanky et al. Computational Materials Science, 162(2019)

Those properties make it an ideal candidate for use in many applications – once we better understand its behavior under various conditions.

Researchers have been looking at the many applications of graphene since it was first isolated in 2004. It is already used in tennis rackets and bicycle wheels. Another area of potential use, however, is drug delivery, which was the focus of a study conducted by researchers at the New Jersey Institute of Technology (NJIT) that was recently published in the *Computational Materials Science* journal.

NJIT Mechanical and Industrial Engineering Professor Dibakar Datta and his team used the *Comet* supercomputer at the San Diego Supercomputer Center (SDSC), located at the University of California San Diego, to create detailed simulations of graphene-water interactions to determine if graphene is a good candidate for delivering medicine to a specific part of the body.

While graphene has been extensively studied for many years in water-based solutions, especially in the biomedical sciences field, researchers say they still need to better predict the surface traits of such two-dimensional materials when exposed to water or liquids containing water.

The findings describe in detail how graphene interacts with a droplet of water. “One of the critical issues is how the graphene flakes behave when they are placed inside a water droplet, said Datta. “Doing experiments to understand the graphene-water interaction is expensive and requires a great deal of labor, so to meet this challenge, we performed computer simulations to gain fundamental insight.”

Researchers found that the graphene flake came out of the droplet to wrap it, which means that graphene is hydrophobic, or adverse to water. There is a particular interest in graphene wrapping for nanocomposite materials, where the wrapped component can be nanoparticles, nanowires, bacteria, and most interestingly the drug. For the drug delivery, graphene flakes and drugs can be placed insight the water droplet. Because of hydrophobicity, all flakes come out and wrap the droplet containing drugs.

Upon the water drying, graphene flakes completely encapsulate the drug and act as a cargo for the drug-delivery applications. Moreover, depending on the arrangements, when multiple graphene flakes were placed inside a water droplet, all of the flakes tended to come out of the droplet and self-assemble, or clump together. This pattern of self-assembly depends upon the size of the water droplet and the geometry of the graphene flakes placed inside it.

The self-assembled graphene can be used for different graphene-based medical nanodevices. Specifically, these simulations showed researchers that by tuning the geometry and the initial arrangement of graphene flakes inside the water droplet, biomedical engineers, physicians, and other medical personnel can utilize the final graphene wrapping or self-assembly for drug-delivery where a water medium is used, and other medical nanodevice applications.

“We also studied how graphene flakes failed when placed inside the droplet,” explained Datta. “Graphene wrinkles to wrap around the water molecules, which means that it doesn’t undergo brittle or sudden breaking or fractures like graphene does in a non-water medium.”

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