'Sticky waves'—molecular interactions at the nanoscale

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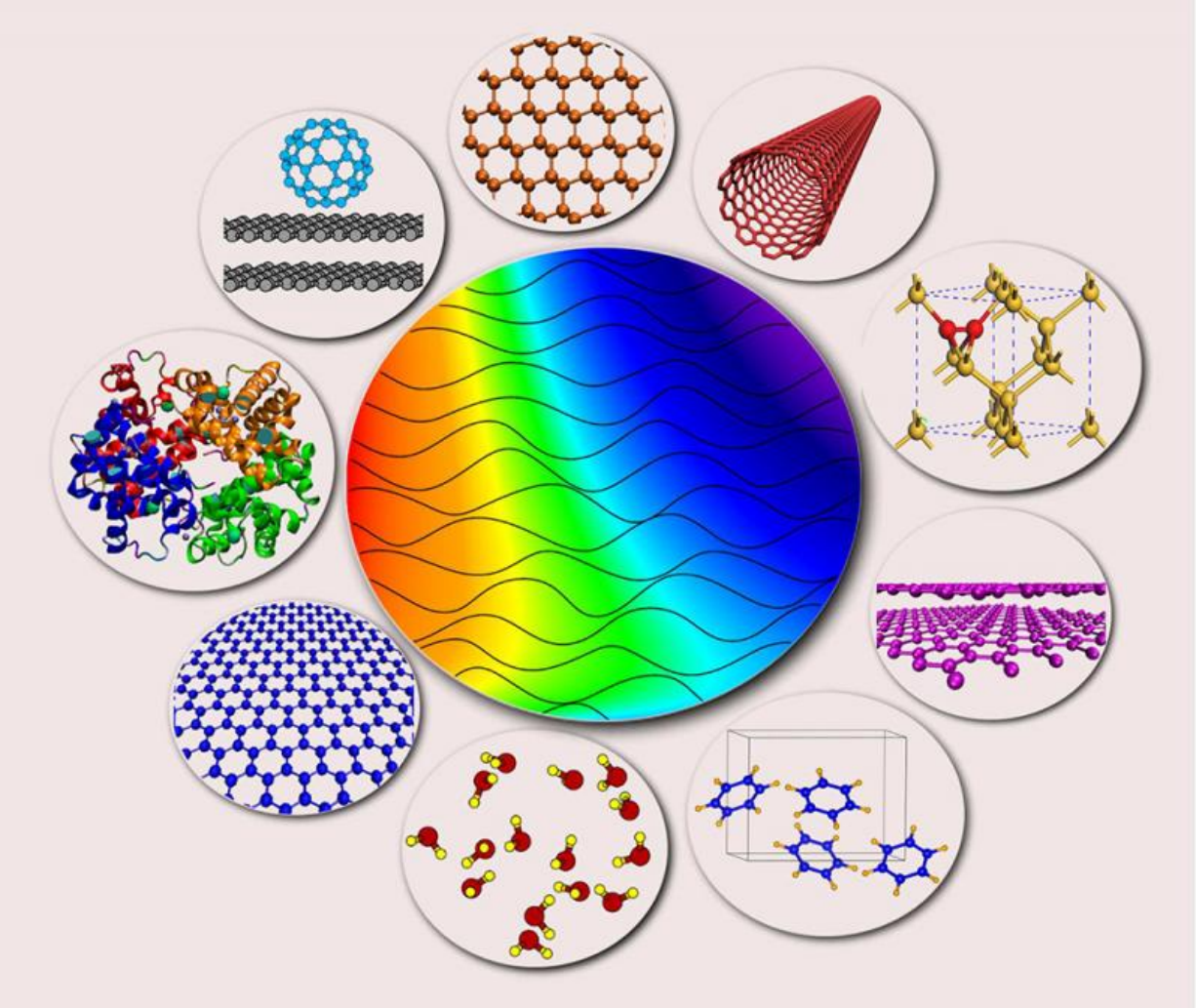

An accurate description of the van der Waals forces between objects at the nanoscale must account for the electrostatic interactions between wavelike charge density fluctuations. These forces are ubiquitous in nature and influence the chemical and physical properties of systems throughout chemistry, biology,

physics and materials science. Credit: Robert DiStasio/Alexandre Tkatchenko

Like the gravitational forces that are responsible for the attraction between the Earth and the moon, as well as the dynamics of the entire solar system, there exist attractive forces between objects at the nanoscale.

These are the so-called van der Waals forces, which are ubiquitous in nature and thought to play a crucial role in determining the structure, stability and function of a wide variety of systems throughout the fields of biology, chemistry, physics and materials science.

"To put it simply, every molecular system and every material in nature experiences these forces," said Robert A. DiStasio Jr., assistant professor of chemistry and chemical biology in the College of Arts and Sciences. "In fact, we are finding that their influence is quite extensive, and includes protein-drug interactions, the stability of the DNA double helix, and even the peculiar adhesion properties of the gecko's foot."

When compared with the covalent bond (which involves the sharing of electron pairs between atoms), van der Waals forces are relatively weak and arise from instantaneous electrostatic interactions between the fluctuating electron clouds that surround microscopic objects. However, these forces are still quantum mechanical in origin and have posed a substantial challenge for both theory and experiment to date.

In a paper in the March 11 issue of *Science*, DiStasio and collaborator Alexandre Tkatchenko of the University of Luxembourg and the Fritz Haber Institute have put forth a new proposition for describing van der Waals forces among objects at the nanoscale.

Generally speaking, there are two schools of thought regarding these forces. The prevailing description of van der Waals interactions among most chemists and biologists is the picture of two induced electric dipoles, similar to the N and S poles of a magnet, representing the uneven distributions of positive and negative charges. The picture espoused by many physicists, however, centers around the fact that wavelike vacuum fluctuations are responsible for the van der Waals interactions among larger macroscopic objects.

In their work, DiStasio and Tkatchenko demonstrate that these fundamental forces between nanostructures must also be described by the electrostatic interactions between wavelike (or delocalized) charge density fluctuations instead of the aforementioned particle-like (or local) induced dipoles. They believe their work could help to bridge the gap between these two belief systems, and help scientists understand and control the interactions between objects at the nanoscale.

"Our work is demonstrating that there is a much wider variety of systems, such as nanostructured systems, where you have to think about the van der Waals force in terms of interactions between waves instead of interactions between particles," Tkatchenko said.

Paul McEuen, the John A. Newman Professor of Physical Science and director of the Kavli Institute at Cornell for Nanoscale Science, sees the duo's research as an important first step in a long, complicated journey to what McEuen half-jokingly characterized as "solving biology."

"It sounds like a rather boring problem, but it's actually a deeply important problem, the way biomolecules assemble and so on," said McEuen. "It's a hugely important problem, especially for someone like me, who's a nano-guy, but it's going to take time to solve."

McEuen is excited about the work, and said he and DiStasio are

expecting to collaborate on related research in the future.

"This work provides a conceptual framework, or common language, that biologists, chemists, physicists and materials scientists can use to describe van der Waals forces at the nanoscale," DiStasio said. "It also provides a computational framework for accurately predicting how these ubiquitous interactions influence the physical and chemical properties of matter."

More information: A. Ambrosetti et al. Wavelike charge density fluctuations and van der Waals interactions at the nanoscale, *Science* (2016). DOI: 10.1126/science.aae0509

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