# Researchers refute textbook knowledge in molecular interactions

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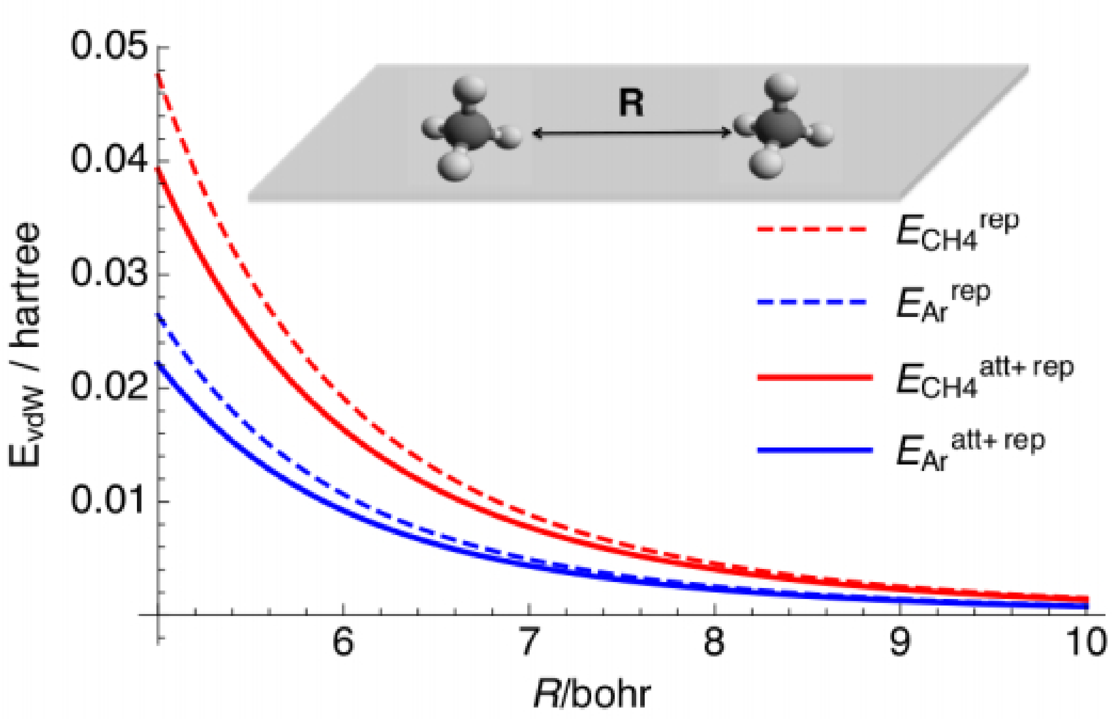


Repulsive ground state interaction E rep (solid lines) and the sum of repulsion and London attraction (E att) energy (broken lines) for argon and methane dimers on a perfectly reflecting surface. Credit: arXiv:1610.09275 [cond-mat.mes-hall]

Van der Waals interactions between molecules are among the most important forces in biology, physics, and chemistry, as they determine the properties and physical behavior of many materials. For a long time, it was considered that these interactions between molecules are always attractive. Now, for the first time, Mainak Sadhukhan and Alexandre Tkatchenko from the Physics and Materials Science Research Unit at the University of Luxembourg found that in many rather common situations in nature the van der Waals force between two molecules becomes repulsive. This might lead to a paradigm shift in molecular interactions.

"The textbooks so far assumed that the forces are solely attractive. For us, the interesting question is whether you can also make them repulsive," Prof Tkatchenko explains. "Until recently, there was no evidence in scientific literature that van der Waals forces could also be repelling." Now, the researchers have shown in their paper, published in the renowned scientific journal *Physical Review Letters*, that the forces are, in fact, repulsive when they take place under confinement.

The ubiquitous van der Waals force was first explained by the German-American physicist Fritz London in 1930. Using quantum mechanics, he proved the purely attractive nature of the van der Waals force for any two molecules interacting in free space. "However, in nature molecules in most cases interact in confined spaces, such as cells, membranes, nanotubes, etc. In is this particular situation, van der Waals forces become repulsive at large distances between molecules," says Prof Tkatchenko.

Mainak Sadhukhan, the co-author of the study, developed a novel quantum-mechanical method that enabled them to model van der Waals forces in confinement. "We could rationalize many previous experimental results that remained unexplained until now. Our new theory allows, for the first time, for an interpretation of many interesting phenomena observed for molecules under confinement," Mainak Sadhukhan says.

The discovery could have many potential implications for the delivery of pharmaceutical molecules in cells, water desalination and transport, and self-assembly of molecular layers in photovoltaic devices.

Prof Tkatchenko's research group is working on methods that model the properties of a wide range of intermolecular interactions. Only in 2016, they found that the true nature of these van der Wals forces differs from conventional wisdom in chemistry and biology, as they have to be treated as coupling between waves rather than as mutual attraction (or repulsion) between particles.

**More information:** Mainak Sadhukhan et al, Long-Range Repulsion Between Spatially Confined van der Waals Dimers, *Physical Review Letters* (2017). DOI: 10.1103/PhysRevLett.118.210402 , arxiv.org/abs/1610.09275

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