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Van der waals interaction between nanostructures

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Abstract

Van der Waals (vdW) interaction is an important quantum many-body effect arising from long-range correlation. While it is only about 1% of normal chemical bond, it affects many properties of materials. A good understanding of this effect may benefit many branches of science (such as chemistry, physics, materials science, biology, etc.) and technology (such as hydrogen storage, catalyst preparation, and physical purification). However, the vdW interaction between large (many-atom) systems cannot be entirely captured with first-principles calculations, due to computational challenges. In this talk, I will discuss a simple model for the dynamic multipole polarizability, from which vdW coefficients between nanoclusters can be accurately generated. Analysis of the size dependence of vdW coefficients with this model leads to an important discovery: An old but still the most widely-used “atom pair wise interaction picture" surprisingly breaks down for most nanoclusters. A quick remedy of this problem leads to a counterintuitive scaling law of the vdW coefficients for clusters that allow for a cavity, such as fullerenes.

Biography

Dr. Jianmin Tao is a Research Assistant Professor in Physics Department of Tulane University. He received M.S. degree in chemical physics from University of Science and Technology of China in 1988, and Ph. D. degree in physics from Tulane University in 2002. Dr. Tao has broad research interests, including density functional theory, quantum many-body dynamics, and van der Waals interaction. He has published 60 papers in peer-reviewed journals and one of his papers (first author) has been cited over 1200 times.