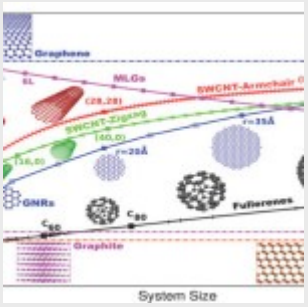
Non-Covalent van der Waals Interactions at the Nanoscale: A Solved Problem?



Title: Non-Covalent van der Waals Interactions at the Nanoscale: A Solved Problem?
When: Thursday, 14 April (2016), 15:00h
Place: Departamento de Física Teórica de la Materia Condensada, Facultad Ciencias, Module 5, Seminar Room (5th Floor).
Speaker: Prof. Alexandre Tkatchenko, Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg.

Non-covalent van der Waals (vdW) interactions are ubiquitous in molecules and materials. The influence of vdW forces extends well beyond binding energies and encompasses the structural, mechanical, spectroscopic, and even electronic signatures of molecular systems and condensed matter. Our conceptual understanding of these interactions is largely based on perturbative models, which are often unable to capture the full extent of non-local quantum-mechanical fluctuations which can extend up to tens of nanometers in real systems [1]. The origin of such many-body fluctuations will be discussed and their importance demonstrated for a hierarchy of systems, ranging from simple gas-phase dimers, supramolecular host-guest complexes, extended molecular crystals, to layered 2D heterostructures. The development of efficient many-body methods that explicitly address the non-local collective nature of quantum fluctuations not only leads to significant improvements in the accuracy of calculations [2,3,4], but also allows us to discover novel conceptual insights that give us the ability to control these fluctuations in the design of intricate materials. These facts will be highlighted by presenting a few selected examples from our recent work [3,4].

References

A. Ambrosetti, N. Ferri, R. A. DiStasio Jr., and A. Tkatchenko, Science 351, 1171 (2016).
A. Tkatchenko, R. A. DiStasio Jr., R. Car, and M. Scheffler, Phys. Rev. Lett. 108, 236402 (2012).
A. Tkatchenko, Adv. Func. Mat. 25, 2054 (2015).
A. M. Reilly and A. Tkatchenko, Chem. Sci. 6, 3289 (2015).

More information on IFIMAC Website