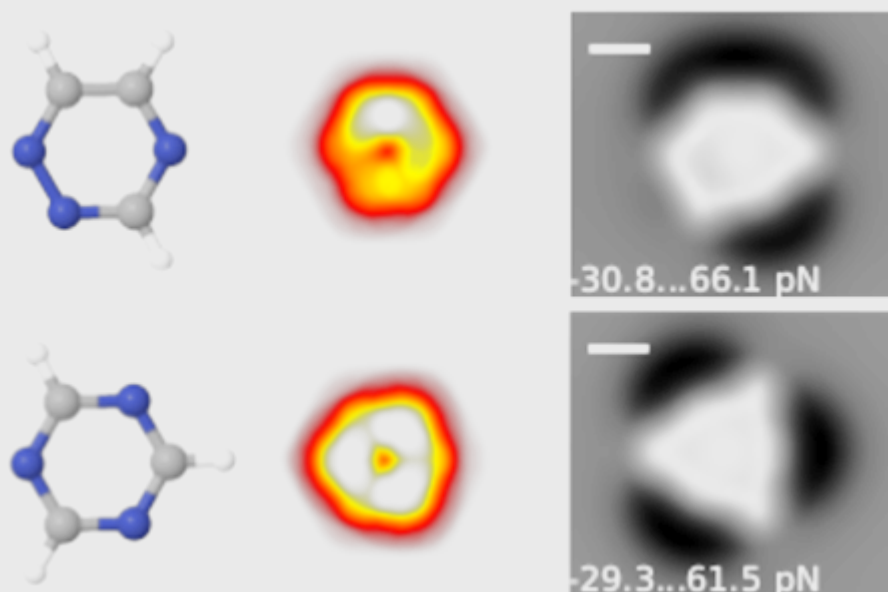


## Molecular Identification and Bonding Information from High-resolution AFM



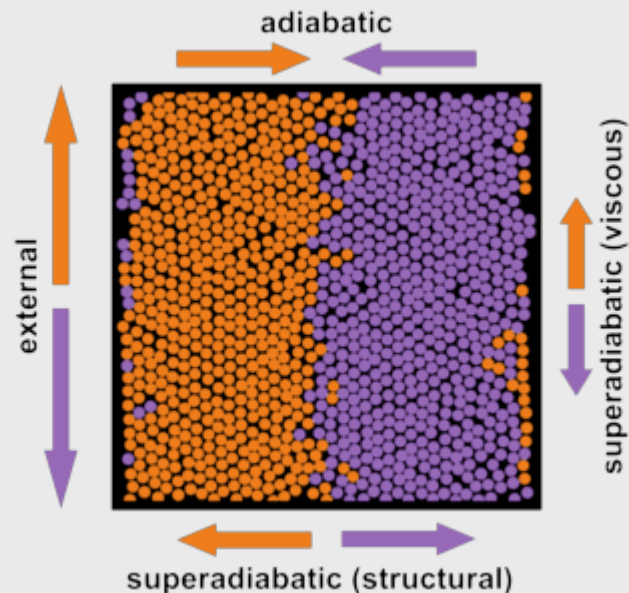
Article: published in [ACS Nano](#) by Pablo Pou and Ruben Perez, [IFIMAC](#) researchers and members of the Department of Theoretical Condensed Matter Physics.

**H**igh-resolution atomic force microscopy (HR-AFM) is able to image the internal structure of molecules, resolves features in the intermolecular regions of weakly bonded molecules, discriminates between bond orders in aromatic compounds, and has opened the door to following or even inducing on-surface chemical reactions. This revolution in molecular imaging has sparked a strong debate about the interpretation of the experiments and the development of new capabilities like chemical identification. Here, we introduce an efficient method to simulate HR-AFM images with CO probes. Our model explicitly takes into account the charge densities of the sample and the probe for the calculation of the short-range (SR) interaction and retains *ab initio* accuracy with only two parameters, that are essentially universal, independent of the number of chemical species and the complexity of the bonding topology. The application to molecular images shows a strong dependence on the stoichiometry and bonding configuration that precludes the chemical identification of individual atoms based on local force-distance curves. However, we have identified features in the 2D images and 3D force maps that reflect the highly anisotropic spatial decay of the molecular charge density and provide a way towards molecular identification. The model treats SR and electrostatics interactions on an equal footing and correctly pinpoints the Pauli repulsion as the underlying interaction responsible for the bond order discrimination in C60. Finally, we settle the controversy regarding the origin of the intermolecular features, discarding the effect of the charge redistribution associated with the H bonds, and linking them with the overlap of the wave functions of the atoms that constitute the bond. This overlap creates saddle regions in the potential energy landscape that are

sensed by the probe. [[Full article](#)]

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## Velocity Gradient Power Functional Theory for Brownian Dynamics



Title: Velocity Gradient Power Functional Theory for Brownian Dynamics.

When: Wednesday, November 27, (2017), 12:00.

Place: Department of Theoretical Condensed Matter Physics, Faculty of Science, Module 5, Seminar Room (5th Floor).

Speaker: Daniel de las Heras, Theoretische Physik II, University of Bayreuth, Germany.

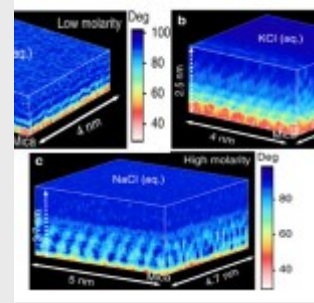
# P

ower functional theory is an exact generalization of equilibrium density functional theory to nonequilibrium Brownian dynamics. We present an explicit and simple approximation for the superadiabatic excess (over ideal gas) power functional based on the local velocity gradient. The resulting superadiabatic forces, obtained via functional differentiation, are beyond dynamical density functional theory and explain a broad range of phenomena such as viscous forces, lane formation in colloidal systems, and shear migration.

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[Atomically Resolved Three-dimensional Structures of Electrolyte Aqueous Solutions Near a Solid Surface](#)

Article: published in [Nature Communications](#) by [Pedro Tarazona](#), Department of Theoretical Condensed Matter Physics and IFIMAC researcher.



In a collaboration with experimental and theoretical groups of the ICMM-CSIC and IFIMAC-UAM, this paper presents novel experimental results obtained with a three dimensional atomic force microscopy scanning (3D-AFM) taken within a salt-water solution near a mica surface. The atomic resolution of the 3D-AFM uncovers a crystal like structure within the liquid, which propagates from the mica, in structured layers, up to several nanometers. The theoretical analysis, based on a classical density functional description of the liquid mixture, provides the hints to understand a phenomenon which may be of relevance in a large variety of fields, from surface electrochemistry to molecular and cell biology. [\[Full article\]](#)

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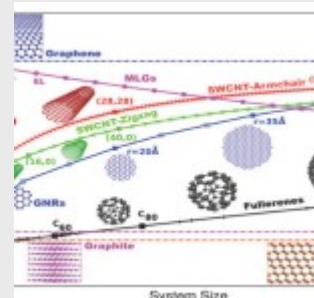
## Non-Covalent van der Waals Interactions at the Nanoscale: A Solved Problem?

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](#)

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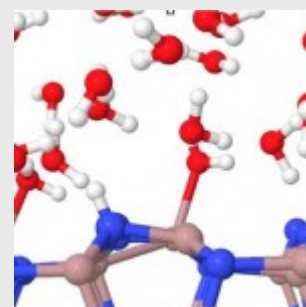
### First Principles Understanding of Liquid Water and its Anomalies

Title: First Principles Understanding of Liquid Water and its Anomalies

When: Tuesday, 22 December (2015), 12:00h

Place: Departamento de Física de la Materia Condensada, Facultad de Ciencias, Module 3, Seminar Room (5th Floor).

Speaker: Marivi Fernandez-Serra, Physics & Astronomy department, Stony Brook University, New York, USA.



**S**urprising as it might seem, the understanding of the structure of liquid water is still an open subject, one that has kept theorists and experimentalists busy for the last 50 years. One of the reasons for this is the fact that water is a liquid with a large number of thermodynamical anomalies, and no single theoretical model is capable of explaining them all, or of reproducing all experimental measurements conducted to probe its structure. Advanced computational modeling needs to be developed to simulate the structure and dynamics of liquid water. In this talk, I will show how recent advances within the framework of density functional theory have allowed us to understand the physics behind some of the anomalies of water. Our research indicates that the structure and dynamics of liquid water are not so different from its solid phase. In particular, I will show that the hydrogen bond network of water supports propagating

optical phonon-like modes.

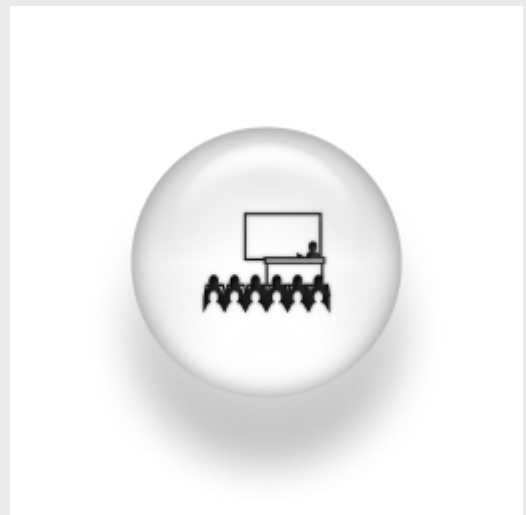
We argue that on subpicosecond time scales these modes propagate through water's hydrogen bond network over distances of up to two nanometers. In the long wavelength limit these optical modes exhibit longitudinal-transverse splitting, indicating the presence of coherent long range dipole-dipole interactions, as in ice. Our results indicate the dynamics of liquid water have more similarities to ice than previously thought.

[More information on IFIMAC Website](#)

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## Density Functional Theory - OpenMX

Thursday, 7 April 2011, 12:00-13.00



*Prof. Taisuke Ozaki*

Japan Advanced Institute of Science and Technology (JAIST)

ABSTRACT:

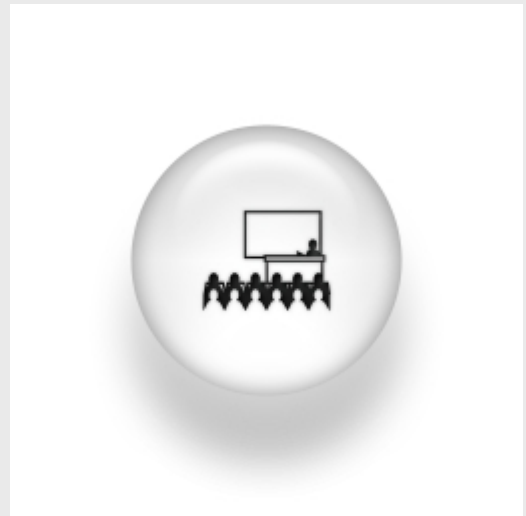
During the last three decades continuous efforts have been devoted to extend applicability of the density functional theory (DFT) to large-scale systems, leading to realization of more realistic simulations close to experimental conditions. In this talk, I will introduce our recent developments of low-order scaling methods for eigenvalue problem and evaluation of exact exchange energy towards the direction [1-5]. It is demonstrated that a linear-scaling Krylov subspace method [1], combined with effective screening medium (ESM) method [6], enables us to simulate a bias induced chemical reaction in lithium battery. Moreover, a numerically exact low-order scaling method is presented [2,3], which directly evaluates selected elements of density matrix using a nested dissection approach. Finally, an exchange functional by a range-separated exchange hole, whose computational cost is linear-scaling, is proposed to calculate the exact exchange energy [4]. I will also summarize the OpenMX project [5] in an east Asian community to develop a platform for large-scale DFT simulations.

[1] T. Ozaki, PRB 74, 245101 (2006).

- [2] T. Ozaki, PRB 75, 035123 (2007).  
[3] T. Ozaki, PRB 82, 075131 (2010).  
[4] M. Toyoda and T. Ozaki, PRA, in press.  
[5] <http://www.openmx-square.org/>  
[6] M. Otani and O. Sugino, PRB 73, 115407 (2006).
- 

## Intermolecular interaction in DFT : Application to Carbon Nanotubes and Fullerenes

Wednesday, 4 March 2009, 12:00-13.00



*Dr. Y.J. Dappe*

Institut de Physique et Chimie des Matériaux de Strasbourg

### ABSTRACT:

A theoretical study of weak interactions in graphitic materials like Carbon Nanotubes, Fullerenes and graphene is presented here. Based on a localized orbitals DFT formalism, our treatment which has already been applied for graphene-graphene interaction describes independently the weak chemical as well as the van der Waals interaction with high accuracy. The weak chemical interaction is described in the frame of the LCAO-S2 model based on a weak overlap expansion, and the van der Waals interaction is treated in the dipolar approximation, taking into account virtual transitions of high energy. This formalism is applied here to the case of lateral interaction between CNTs, C60-dimers, adsorption of C60 on graphene and CNT, and encapsulation of C60 and CNT. The power law of the interaction is analyzed, and useful parameters like C60 coefficient and an exponential model for the “chemical” interaction are extracted. Beyond the study of graphitic materials, this work opens new perspectives in the analysis of weakly bounded metal/organics interfaces.

M.A. Basanta, Y.J. Dappe, J. Ortega and F. Flores, Europhysics Letters 70, 355 (2005).

Y.J. Dappe, M.A. Basanta, F. Flores and J. Ortega, Physical Review B 74, 205434 (2006).

Y.J. Dappe, J. Ortega and F. Flores, submitted to Physical Review B (2008).

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