Power 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.
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]
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

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.

Surprising 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 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

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.

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.
