

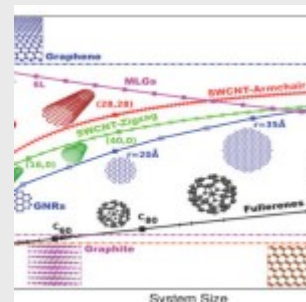
## Non-Covalent van der Waals Interactions at the Nanoscale: A Solved Problem?

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.



**N**on-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

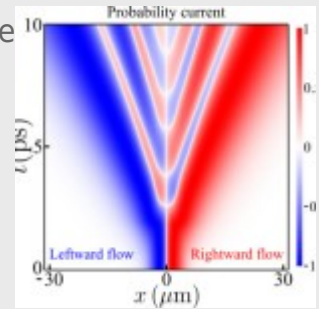
- A. Ambrosetti, N. Ferri, R. A. DiStasio Jr., and A. Tkatchenko, *Science* 351, 1171 (2016).
- A. Tkatchenko, R. A. DiStasio Jr., R. Car, and M. Scheffler, *Phys. Rev. Lett.* 108, 236402 (2012).
- A. Tkatchenko, *Adv. Func. Mat.* 25, 2054 (2015).
- A. M. Reilly and A. Tkatchenko, *Chem. Sci.* 6, 3289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

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### Self-Interfering Wave Packets

Article: published in [Physical Review Letters](#) by David Colas and [Fabrice P. Laussy](#),



The Schrödinger wave packet is a fundamental concept of quantum mechanics that, historically, gives the probability (amplitude) to find a particle at a particular position (or a particular momentum, one excluding the other). Gaussian wave packets are natural solutions of the Schrödinger equation, and their dynamical properties (diffusion, scattering against a potential, etc...) are well known by graduate physics students. Many kinds of wave packets and their connections to particles have since been discovered, such as solitons, that can maintain their shape through propagation if interactions between particles are present, or the Airy beams discovered by Berry and Balazs, that accelerate without any external force or interactions.

We add another member to the family of noteworthy non-interacting wave packets. Taking advantages of the nonlinear dispersion relation of polaritons—quasiparticles arising in semiconductor microcavities from the coupling of a light field (cavity photons) and a matter fields (excitons of a quantum well)—we demonstrate theoretically that a simple Gaussian pulse can give rise to a Self-Interfering Wave Packet (SIP) that exhibits solitonic properties, although non-interacting. This is powered by the polaritonic dispersion that provides diffusive effective masses of different signs within the same wave packet, leading to self-interferences. A rich phenomenology arises from this concept, such as adding Rabi oscillations that order a spacetime crystal, or by detuning the system which produces ultrafast subpackets. [\[Full article\]](#)

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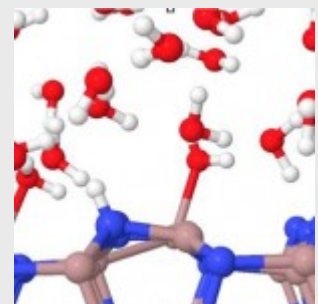
## First Principles Understanding of Liquid Water and its Anomalies

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.

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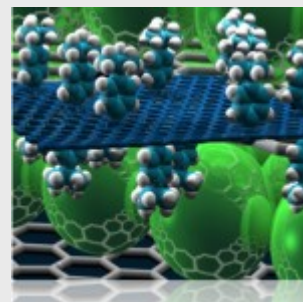
## [Exfoliation, Hybridization and Chemical Functionalization of 2D Materials](#)

Title: Exfoliation, Hybridization and Chemical Functionalization of 2D Materials

When: Friday, 18 December (2015), 15:00h

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

Speaker: Gonzalo Abellán, Institute of Advanced Materials and Processes (ZMP), University Erlangen-Nuremberg, Fürth, & Department of Chemistry and Pharmacy, University Erlangen-Nuremberg, Erlangen, Germany.



**R**ecently, graphene (G) and related 2D materials have attracted a considerable attention due to their appealing electronic properties and the possibility to be tailored

by chemical modification. In this sense, the efficient exfoliation of these building blocks is of utmost importance for its subsequent derivatization. Moreover, the formation of hybrid materials based on 2D building blocks have found many applications because they allow combining the properties of inorganic solids such as robustness, durability or mechanical strength with those introduced by the organic component such as functionality, tunability and convenient functionalization by synthesis.

Herein we will discuss several routes developed in our labs towards the exfoliation, hybridization into complex systems and chemical functionalization of three 2D materials, namely layered double hydroxides (LDH), graphene and black phosphorus –the newest member of the 2D family. Finally, some interesting applications will be presented.

G. A. thanks the EU for a Marie Curie Fellowship (FP7/2013-IEF-627386).

#### References

- G. Abellán et al., Acc. Chem. Res., 2015, 48, 1601.
- G. Abellán et al., Adv. Mater. 2014, 26, 4156.
- G. Abellán et al., Chem. Sci. 2015, 6, 1949.
- G. Abellán et al., Chem. Commun. 2015, 51, 14207.
- G. Abellán et al., J. Mater. Chem. C, 2014, 2, 3723.
- G. Abellán et al., ES Patent WO2013124503 A1.
- D. Hanlon et al., Nature Commun. 2015, 6, 8563.

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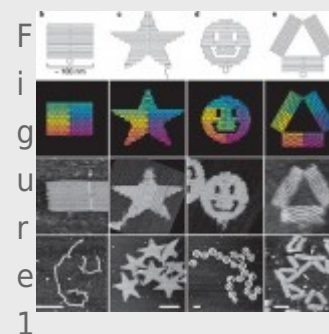
## Building Nano-Lenses Based on DNA Origami Structures

When: Friday, 20 November (2015), 12:00h

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

Speaker: Guillermo Acuña, TU Braunschweig, Institute of Physical and Theoretical Chemistry, Hans-Sommer-Str. 10, Braunschweig, Germany.

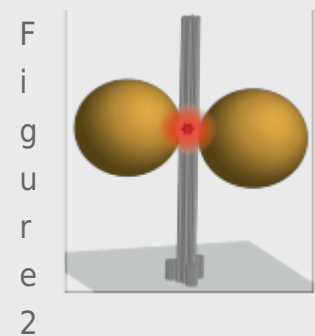
Abstract:



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In this presentation, we will show how the DNA-Origami technique [1] (Figure 1.) can be introduced for plasmonic and photonic applications. Firstly, we employ DNA-Origami as a platform where metallic nanoparticles as well as single organic fluorophores can be organized with nanometer precision in three dimensions. With these hybrid structures we initially study the nanoparticle-fluorophore interaction in terms of the distance-dependent fluorescence quenching [2] and angular dependence around the nanoparticle [3]. Based on these findings, we build highly efficient nano-lenses (Figure 2.) based on 100 nm gold dimers [4] which are able to strongly focus light into the sub-wavelength region where the fluorophore is positioned and produce a fluorescence enhancement of more than two orders of magnitude [5].



Using this highly confined excitation field we were able to perform single molecule measurements in solution at concentrations as high as 25 $\mu$ M in the biologically relevant range. Additionally, we report on a controlled increment of the radiative rate of organic dyes in the vicinity of gold nanoparticles with the consequent increment in the number of total emitted photons [6,7].

#### References

- P. W. Rothmund, Nature 440, (2006) 297.
- G. P. Acuna et al., ACS Nano 6, (2012) 3189.
- F. Möller, P. Holzmeister, T. Sen, G. P. Acuna and P. Tinnefeld, Nanophotonics 2, (2013) 167.
- G. P. Acuna et al., Science 338, (2012) 506.
- A. Puchkova et al., Nano Letters, just accepted (2015).
- J. Pellegrotti et al., Nano Letters 14, (2014) 2831.
- P. Holzmeister, E. Pibiri, J.J. Schmied, T. Sen, G. P. Acuna and P. Tinnefeld, Nat. Comm. 5, (2014) 5356.

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