DEPARTAMENT DE FÍSICA I ENGINYERIA NUCLEAR *NUMBER 17, AUTUMN 2014*

FENOMEN

NEWSLETTER OF THE PHYSICS AND NUCLEAR ENGINEERING DEPARTMENT

NEWS

AWARDS

Julio Garcia-Martinez, former GCM PhD student, has received the PhD award to the best PhD thesis in the Science area.

Vito Roppo, former DONLL PhD student, has received the extraordinary PhD award.

Jordi Boronat has been elected as APS Fellow for 2014 in the Division of Computational Physics.

SPECIAL PUBLICATIONS

Special Issue in the **Journal Non-Crystalline Solids** – selection of invited papers at the 7th IDMRCS Conference, organized in July 2013 at Barcelona.

http://www.sciencedirect.com/science/journal/00223093/407. **Guest Editors:** S. Capaccioli, K.L. Ngai, G. Ruocco and J.L. Tamarit

INVITED RESEARCHERS

Mattwiew Asamoah, researcher of Ghana Atomic Energy Agency granted by the International Atomic Energy Agency (IAEA) - "sanchiw" research mobility at NERG.

Prof. Wieslaw Krolikowski, director of the Laser Physics Center, Research School of Physics and Engineering, Australian National University, Canberra, Australia (invited professor at DONLL).

NEW GRANTED PROJECTS

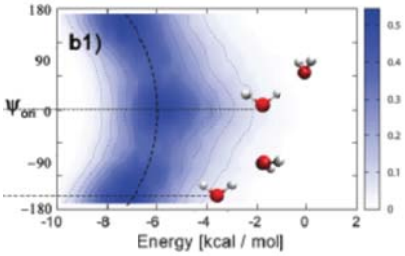
"Vidrios orgánicos y metálicos: estructura, dinámica y estabilidad" (FIS2014-54734-P, granted by MICINN (red de excelencia)
PI: J.L. Tamarit
Participants: Univ. Pais Vasco, Univ. Complutense de Madrid, Univ. Autónoma de Madrid, Univ. Autónoma de Barcelona, and Univ. Politècnica de Catalunya.

RECENT PUBLICATIONS

Chemical Physics

Liquid water: a continuous mixture of two different dimers

It is hitherto thought that liquid water is composed of tetrahedral coordinated molecules with an asymmetric interaction of the central molecule with neighboring molecules. In order to investigate the geometric origin of that asymmetry, a collaboration between researchers of GCM and SIMCON (L. C. Pardo, A. Henao, S. Busch, E. Guardia and J. Ll. Tamarit), scrutinized molecular dynamics (MD) simulations of water through a careful analysis of the five-dimensional probability distribution function of Euler angles in which the relative positions and orientations of water molecules are obtained.

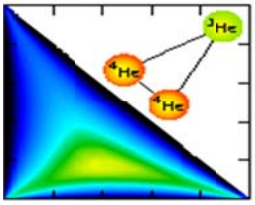


They demonstrated that, beyond the ubiquitous tetrahedral structure with well-defined molecular dimers, there is a series of possible molecular orientations that define the structure. These orientations are generated by rotating the neighboring molecule around the O–H axis that is involved in the hydrogen bond scheme. Two of the possible orientations have a higher probability, giving rise to two kinds of dimers: one close to the lowest energy of a water dimer in vacuum with an almost perpendicular alignment of the dipole moment, and another one with a parallel orientation of the dipole moment which is less tightly bound. ***(Phys. Chem. Chem. Phys. 16, 24479, 2014)***.

Molecular physics

Universality in molecular halo clusters

Universality is important in nearly all areas of physics, since it enables the establishment of connections between phenomena at different energy and length scales. It is also a key characteristic of quantum halo states, usually defined as bound states which extend far into the classically forbidden regions. In a recent collaboration, J. Boronat from Barcelona Quantum Monte Carlo (BQMC) group and researchers of the University of Split in Croatia, universality of the properties of dimers and trimers with halo character has been established for the first time using quantum Monte Carlo methods.

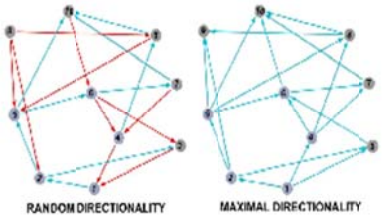


By a proper definition of scaled size and energy all halo states follow the same law independently of the specific shape of the interaction. It is remarkable, and probably unexpected, that the universal law extends even significantly below the halo limit for both dimers and trimers. (***Phys. Rev. Lett. 113, 253401, 2014***).

Complex Networks

Hierarchy and Loops

Many biological systems, ranging from food webs to cell metabolism, can be represented as directed networks. A puzzling common feature of these systems is the lack of directed loops: in nearly all biological networks, one observes much fewer directed loops than in random networks. S. Pigolotti from DONLL, in collaboration with colleagues from University of Granada, provided a simple mathematical explanation for this finding.



The theory is based on the presence of a hierarchy of nodes, representing for example increasing body mass in food webs. The distribution of number of directed loops, that can be analytically computed within this theory, agrees very well with experimental data. (***Scientific Reports 4, 7497, 2014***).

The Nobel laureates in Physics and Chemistry 2014

In 2014, the Nobel Prizes in Physics and Chemistry have been awarded to scientists that work in subjects related with photonics, which is a good precursor for the International Year of Light, 2015. They address applied issues rather than fundamental ones.

The Nobel Prize in Physics 2014 was awarded jointly to **Isamu Akasaki, Hiroshi Amano** and **Shuji Nakamura** ***"for the invention of efficient blue light-emitting diodes which has enabled bright and energy-saving white light sources".***

Light-emitting diodes (LEDs) are very efficient and fast-response light sources that are progressively substituting other light sources in fields such as lighting, color displays, sensors, etc. This might allow humanity to save a lot of energy and to make more efficient devices for different purposes. For most of these applications (lighting, color displays,…) emission at different wavelengths is needed. For instance, for the emission of white light, or for controlling the color, it is well known that emission at least at red, green and blue colors (RGB) is needed. In a LED, however, each color requires use of a different semiconductor material (with a different gap energy), as the color is determined by the emission frequency, which is given by the energy gap. These energy gaps, on the other hand, must be "direct", for the light emission efficiency to be large.

GaAs was the first one which emits in the infrared. Soon later red emission could be achieved with an alloy of III-V materials, and later some emitters in green or blue were achieved, but their efficiency and durability was not satisfactory for massive applications and high-power emission. The three Nobel Prizes contributed to the fabrication of efficient, robust and durable enough semiconductors that can emit in the blue or even in UV. These materials involve N, a component that is difficult to mix with the other components to get stable enough structures, but they succeeded to find an appropriate growth process. With blue light it is also possible, nowadays, to get white light (and thus to get white LEDs for lighting purposes), as the blue light has a frequency large enough to pump other materials (ceramic materials such a cerium, Ce) and get emission in a wide domain of lower frequencies, which covers almost all the visible spectrum.

The Nobel Prize in Chemistry 2014 was awarded jointly to **Eric Betzig, Stefan W. Hell** and **William E. Moerner** ***"for the development of super-resolved fluorescence microscopy"***

As it is well known, the resolution of a standard optical microscope is limited by diffraction, so that the minimum object that can be clearly seen or distinguished is of size of the order of the light wavelength (the best classical optical microscope, the confocal one, has a resolution of ca. 200 nm, using blue light, which has the smallest wavelength in the visible spectrum).

In medicine and biology, however, many constituent elements and dynamic processes occur at smaller spatial scales (be it around or inside a cell, nerves, bacteria, viruses, cell expression, DNA and related molecules, proteins, …). In the last decades, new microscopy methods have been implemented, which take advantage of the light emitted, by fluorescence, by naturally generated or injected fluorescent molecules or proteins located or attached to different parts of cells (or of other objects), when they are illuminated by light of higher frequency. Nevertheless, the problem of the limited spatial resolution remains, as both the excitation and observation is made by means of light and lenses.

The Nobel Prize winners implemented methods to go beyond this spatial resolution. For instance, Stefan W. Hell invented the STED ("STimulated-Emission Depletion") method, in which the light excitation pulse is immediately followed by a short and intense "depletion" pulse whose transverse structure is in form of a "donought" (i.e, with a dark spot in the center) and whose frequency is smaller and coincides with that of the fluorescence that the biological sample is going to emit. The result is that the incident donought pulse deexcites the fluorescent molecules by stimulated emission, before they initiate the spontaneous emission fluorescence! Only the molecules falling inside the donought hole will remain excited! so that the spatial resolution improves a lot. Details of size as small as 25nm have been observed. Nowadays STED microscopes are being used more and more.

Ramon Vilaseca (DONLL)

PhD THESIS

- **Michele Starnini** "Time-varying network approach to social dynamics: from individual to collective behavior
  Supervisor: R. Pastor, October 9th 2014.
- **Muriel Rovira** "Short range order in disordered phases using neutron diffraction".
  Supervisors: J.L. Tamarit and L.C. Pardo, Sept. 9th 2014.
- **Paula Salvador** "Neutron-induced fission cross section of 240,242Pu"
  Supervisors: C. Pretel, F.J. Hambsch, Nov. 7th, 2014.
- **Victor Martínez** "Scaling-up methodology, a systematical procedure for qualifying NPP nodalizations. Appl. to the OECD/NEA ROSA-2 and PKL-2 Counterpart test"
  Supervisor: F. Reventòs, Nov. 17th, 2014.

NEW PhD STUDENTS

- **Lara Escuain** (J. Garcia Ojalvo and A. Pons).
- **Ali Jasmin Mohammed** (M. Alarcon).
- **Auro Michele Perego** (K. Staliunas)
- **Carlos Quintero** (C. Masoller and C. Torrent).
- **Guadalupe Ruiz** (J.L. Tamarit).
- **Ali Al Nasar** (M. Alarcon).
- **Iduabo John Afa** (C. Serrat)
- **Dorian Gomez** (R. Herrero).
- **Hossam Mohamed Selim** (C. Cojocaru).
- **Antoine Moinet** (R. Pastor).
- **Seyedeh Parsa** (J. Sellares and J. Trull).
- **Alejandra Castedo** (J. Lorca, E. Mendoza).
- **Valentin De Carlos** (F. Fer Caner)
- **Pedro Díaz** (C. Tapia and J. Dies)
- **Marco Fabbri** (A. De Blas and J. Diez)
- **Erika Paola Ramon** (J. Lorca)

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