

# Soft Condensed Matter

## 6 - 1 – Dynamics of gray and dark solitons in the Schrödinger model with time-dependent harmonic potential

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The interaction between solitons formed in Bose-Einstein condensates (BEC) in dilute atomic vapors has been of fundamental interest in the context of its experimental realizations and theoretical studies. We study the collisional dynamics of dark and gray solitons within the mathematical model of the nonlinear Schrödinger equation (NSE) with the time-dependent harmonic potential, which maintains a quasi one-dimensional BEC in an axial confinement field. The exact analytical solutions and numerical experiments reveal many specific features of dark soliton dynamics corresponding to the different experimental conditions. We have found that stable dark-soliton configurations can be formed in the confinement potential independently on a positive or negative sign of non-linearity, contrary to the sign-dependent dynamics of solitons in the absent of a harmonic potential. The oscillation period of the dark solitons coincides with the oscillation period of the harmonic oscillator potential if a dark soliton is formed on a background (the density BEC distribution along the axial coordinate), which oscillates itself in a harmonic trap. On the other hand, in the case of an immobile background, the oscillation period of the black soliton considerable increases because of the periodic transformation of the black solitons to the gray one and vice versa. The soliton become black (it has a maximum depth) at the turning points in the potential because its velocity is zero and gray at the trap center where it has a maximum velocity.

## 6 - 2 – Structural and dynamical properties of water confined between two hydrophilic surfaces

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The properties of water in the vicinity of surfaces and under confinement have been extensively studied during the last years, because of their importance to a quantitative understanding of many processes that not only take place in biological systems, like cells, membranes and microemulsions, but also in many others such as confined water in rocks, ionic channels and interstellar matter. In this work we perform molecular

dynamic calculations of the microscopic structure of TIP5P model water confined between two hydrophilic surfaces and compare with the properties obtained for bulk water within the same model. We calculate the diffusion coefficients and the electronic as well as the atomic density profile of water molecules and polar ions in the system as a function of the number of water molecules per hydrophilic chain ( $n_w$ ). We also study the dependence of the water layer thickness and the effective area per chain molecule with the same parameter.

## 6 - 3 – Swift heavy ion irradiation effects on Carbonyl and trans-vinylene groups in high and low density polyethylene

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Polyethylene is the most widely used polymer and several desirable application properties can be obtained by choosing one of a large variety of its grades. Some works have investigated the local transformations induced by ion-beam irradiation and it has been found that irradiation in polyethylene produces crosslinking, trans-vinylene, end-vinyl, vinylidene and carbonyl groups [1].

In previous works we have studied physico-chemical changes in ultra high molecular weight polyethylene (UHMWPE) due to swift heavy ion irradiation [2]. Fourier Transform Infrared Spectroscopy (FTIR) analysis of the irradiated samples showed that, with different ions, the absorbance of the C=C stretching vibration from trans-vinylene groups containing hydroperoxides presents a maximum at certain ion fluence that is correlated with the electronic stopping power. In other work we found that the decreasing part of the absorbance curve after the maximum is not related to the overall destruction of the polymer that occur at higher fluences [3].

Our purpose was to study the creation and destruction of two functional groups and its relation with material density and ion energy. To this end, we have studied the effects of swift heavy ion irradiation on the physico-chemical modifications of high and low density polyethylene (HDPE and LDPE) irradiated with 47 MeV Li, 12 MeV C and 6.7 MeV He as a function of fluence.

From the FTIR spectra we analyzed the modification on trans-vinylene and carbonyl groups with fluence. Creation and damage cross sections for these groups were compared for three different PE densities.

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# Development of Experimental and Computational techniques

## 7 - 1 - (0001) GaN/RuN short period hexagonal superlattices: A first principles study of structural and electronic properties

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In this work, we investigate the structural and electronic properties of short-period ( $1 \times n$ ) RuN/GaN superlattices (with  $n \leq 4$ ) wurtzite structures in (0001) orientation, using first principle calculations within Density Functional Theory framework (DFT). We employ the Full Potential Linearized Augmented Plane Waves (FP-LAPW) method as implemented in the WIEN2k code. The exchange and correlation effects are treated using the Generalized Gradient Approximation (GGA) of Perdew, Burke and Ernzerhof. In order to determine the best parameters in wurtzite structure, we optimize the total energy as a function of: (i) the unit cell volume, (ii) the  $c/a$  ratio and (iii) the  $z$ -coordinate of Ga and Ru atoms. The  $1 \times 1$ ,  $1 \times 2$ ,  $1 \times 3$  and  $1 \times 4$  superlattices are studied. The unit cell volume, lattice constant and bulk modulus are showed as a function of the period for each superlattice. A detailed studied of the density of states is made and we find that RuN/GaN superlattices present metallic behavior. At Fermi level, the density of states contribution is due to d-like atomic orbitals of Ru

## 7 - 2 - Search of hydrogen transition states through $\alpha$ - and $\beta$ -Fe: The Monomer adapted to first principle calculations

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The presence of hydrogen (H) in solid solution in metals and alloys is due to its small diameter

and its capacity to diffuse with certain facility in the solid state. However, the presence of H in the metal and specifically in steels is in most of the cases not desired, since H alters considerably the mechanical-metallurgical materials properties being them able to fracture. The most classic damage caused by H in steel is the embrittlement. In previous work we study the influence of H in steels by electrochemical techniques and gaseous desorption [1] together with numerical resolution of 2<sup>nd</sup> Fick's law in presence of traps terms. Here a new assessment is employed. In the context of the density functional theory (DFT) we used the ab-initio SIESTA [2] code: based on pseudo-potentials and numeric, atomic-like orbitals. Minimizes the configurational energy using the conjugate gradients technique employing the generalized gradient density approximation (GGA) for exchange and correlation, adapted with a technique recently developed, the Monomer method: technique that finds the potential energy local curvature by using only forces, allowing to march the system towards saddle points, namely, possible activated states between local minima. Here, the energy and forces are provided by SIESTA, which is being used as a subroutine. Our idea is to check the Monomer-SIESTA technique in  $\alpha, \beta$ -FeH systems in comparison with recently available models [4-6]. Proved the method effectiveness, we will dedicate to study the most complex structure of 13%CrFe (bct) related to soft-martensitic steel, very employed in petroleum technology and fusion reactors.

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### 7 - 3 – Study of the magnetic and electronic properties of the $\text{Fe}_4\text{N}$ with pressure

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$\text{Fe}_4\text{N}$  displays a remarkably rich behavior that has attracted the attention of applied as well as basic researchers for as long as 80 years. The earliest interest in the synthesis and study of  $\text{Fe}_4\text{N}$  was motivated by its possible application as a catalyst for the production of ammonia and for its role in the surface treatment of steels with ammonia. Later, its potential as a material for high-density magnetic recording was pointed out and was studied as a component in various thin film devices, due to its high magnetic flux density, low coercivity, low resistance and other suitable properties. This material, like many others, presents a variation of its magnetic properties to apply an external pressure, showing a magnetic structure that has not yet been fully explained.

The  $\text{Fe}_4\text{N}$  has anti-perovskite structure with two distinguishable Fe atoms, an atom occupies the corners of the cubic unit cell,  $\text{Fe}_I$ , and the other in the face center of cubic,  $\text{Fe}_{II}$ , while the N atoms is in the body center.

In the present work, we report *ab-initio* studies about the magnetic properties variations of  $\text{Fe}_4\text{N}$  under pressure where all calculations were performed using Full-Potential Linearised Augmented Plane Wave Method (FP-LAPW) and the exchange-correlation functional were treated using the Perdew-Burke-Ernzerhof functional and Generalized Gradient Approximation (PBE-GGA). Our results show that the magnetic moment of  $\text{Fe}_I$  is almost constant while the magnetic moment of  $\text{Fe}_{II}$  shows an almost discontinuous variation. This is expressed mainly in changing of the electronic structure and specifically in a peculiar behavior of Density of States (DOS), showing a compression of electronic states close to -3eV.

### 7 - 4 – First-principles determination of the nuclear quadrupole moment of the PAC isotope $^{111}\text{Cd}$

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Nuclear methods (such as Mossbauer spectroscopy, or perturbed-angular correlations [PAC], among others) have been extensively applied to study materials to elucidate the (sub)nanoscopic scale environment of impurities or constituent atoms of solids. These techniques are based on the observation of the coupling between nuclear moments and extra-nuclear fields. In the case of electric-quadrupole interactions, the information provided is given as a product of the nuclear quadrupole moment ( $Q$ ), which interacts with the electric-field gradient (EFG) at the nuclear position. This product is proportional to the so-called quadrupole coupling constant frequency  $C_Q$ .

All the information that  $C_Q$  can provide about the system under study could be obtained by confrontation with an accurate prediction of the EFG, such as those obtained with first-principles electronic-structure calculations. Of course, accurate values of the nuclear-quadrupole moments  $Q$  are essential for a correct comparison between the experimentally "determined" EFG and its theoretical prediction. However, for many important probe nuclei, the  $Q$  values are not known or are known with limited accuracy and/or limited precision. This is the case of the  $^{111}\text{Cd}$  isotope. This isotope is the most frequently used tracer in PAC experiments. Although the importance of this isotope, the nuclear quadrupole moment of the sensitive state (the  $5/2^+$  245 keV excited state) is known with limited precision (relative error of 17%). In this work we present a first-principles determination of the nuclear-quadrupole moment of the  $I=5/2^+$  excited state of  $^{111}\text{Cd}$ . This determination was obtained using the common procedure of correlating calculated EFGs and experimentally determined quadrupole coupling constants. Our  $Q$  value [ $Q(5/2^+, ^{111}\text{Cd}) = 0.83(4)$  b] is in excellent agreement with those reported in the literature [ $Q=0.83(13)$  b] but is obtained with largely better precision.