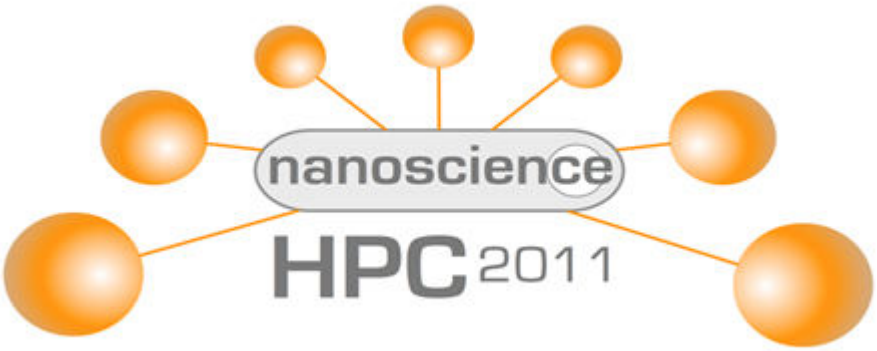
HPC 2011



HPC POSTERS (6)

Parallel software for characterization of large nanostructures using HAADF-STEM

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Atomic resolution High-Angle Annular Dark-Field (HAADF) imaging in scanning transmission electron microscopy (STEM) is rapidly emerging as one of the most important techniques for the characterization of defects in materials. This technique is remarkably sensitive to the atomic number, being possible to generate images of small specimens at sub-Angstrom resolution in aberration-corrected microscopes. As it has been demonstrated recently [1], the measurement of spatial incoherence is important to detect interference effects of electron wave. The effect of spatial incoherence that occurs in electron microscopes produces a significantly lower contrast in experimental images [2]. This effect can be modeled by computer simulation using a convolution of the resulting image with a Gaussian envelope function, but a precise estimation of the incident electron wave is needed to interpret the final Z-contrast images. To maximize simulation precision, an approach to obtain the optimal width of the Gaussian function is presented in this work.

SICSTEM [3] is a parallel simulation software for the simulation of HAADF-STEM images of large nanostructures developed in our research group at the University of Cadiz. SICSTEM runs on a the CAI cluster composed of 80 nodes, each consisting of two Intel Dual Core Xeon 5160 and 8 MB of random access memory, being the overall number of cores equal to 80 x 2 x 2 = 320 and achieving a peak performance of 3.75 TFLOPS (1 TFLOP10^{12} floating point operations per second). It allows the image simulation of large supercells (thousand atoms) within a reasonable time (hours or a few days). SICSTEM takes into account thermal diffuse scattering (TDS) in the calculation of the intensity in the object exit plane by the multislice method using a local TDS absorptive potential approach and its accuracy has been successfully compared to Ishizuka's FFT multislice approach using the WinHREM™ software.

In this work, a new functionality to take into account the effect of spatial incoherence, to reduce the differences in contrast between experimental and simulated images (usually called Stobbs factor) [4] has been included in SICSTEM software. This correction consists on selecting a set of corrected simulated images with different standard deviations and compare them with experimental images using as figure of merit an expression based on the difference in contrast in Fourier space. The proposed functionality aims to be fixed for a given microscope (in the same conditions) and independent of the sample.

In order to show the feasibility of the method and validate its performance, a collection of experimental and simulation images have been used to calculate the effect of spatial incoherence. Experimental images were obtained using a 100kV dedicated VG Microscope HB501Ux STEM equipped with a Nion aberration corrector, Cs = - 50µm, C5 = 63mm, inner detector angle = 70mrad, outer detector angle =

200mrad and objective aperture = 27mrad. In this work, three compositions of InxAs1-xP (27%As, 59%As and 87%As) on a InP substrate and oriented along [110] have been analyzed [5]. For each composition, three different thicknesses have been studied, obtaining a total of nine images. Figure 1 shows error function to determinate the Gaussian function that simulates the effect of spatial incoherence for three As compositions. Figure 2 shows this error function for different thicknesses of InP. From these figures, we might conclude that the proposed method is independent of the composition and thickness of material. Experimental results after the correction have also shown an excellent agreement between simulated and experimental images.

This work was supported by the Spanish MICINN (projects TEC2008-06756-C03- and CONSOLIDER INGENIO 2010 and CSD2009-00013) and the Junta de Andalucía (PAI research groups TEP-120 and TIC-145; project P08-TEP-03516). Work at ORNL was sponsored by the U.S. Department of Energy, Division of Materials Sciences and Engineering (MV and SJP).

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Figures

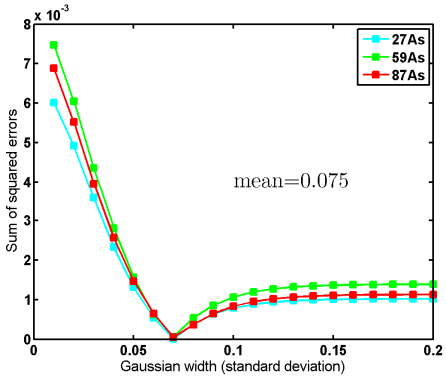

Figure 1.Error function to determine the Gaussian function that simulates the effect of spatial incoherence for three As compositions.

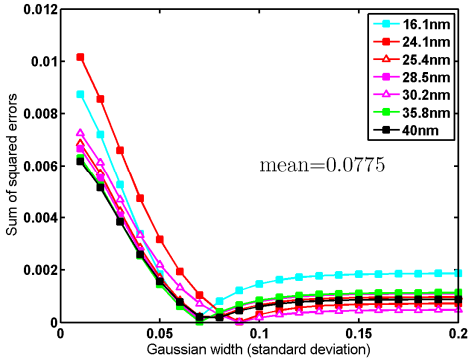

Figure 2.Error function for different thicknesses of InP. It is possible to conclude that the proposed technique is independent of material thickness.

Designing multifunctional chemical sensors using metal doped carbon nanotubes

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We demonstrate a bottom up approach to the computational design of a multifunctional chemical sensor [1,2]. General techniques are employed for describing the adsorption coverage and resistance properties of the sensor based on density functional theory (DFT) and non-equilibrium Green's function methodologies (NEGF), respectively. Specifically, we show how Ni and Cu doped metallic (6,6) single-walled carbon nanotubes (SWNTs) may work as effective multifunctional sensors for both CO and NH_3.

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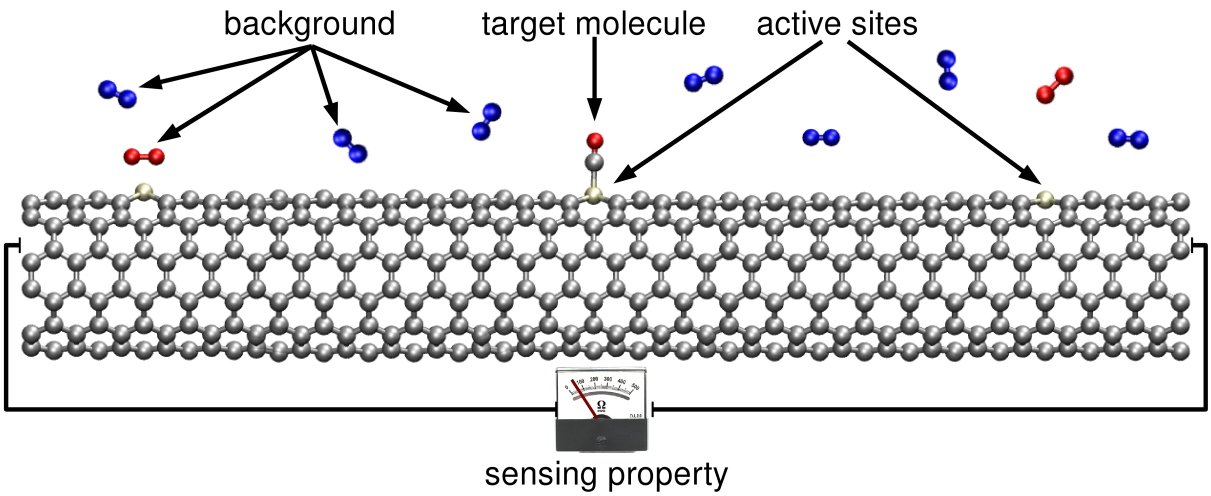

Figure 1: Schematic of a chemical sensor consisting of active sites (metal dopants in a (6,6) carbon nanotube), a target molecule (CO), a background (atmospheric air), and a sensing property (resistance).

FEM simulations on the effect of the thermal-induced surface stress on ultrathin resonators

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Nanoelectromechanical (NEMS) resonators have been developed for use as ultrasensitive sensors including mass sensors, chemical sensors, force sensors and photothermal transducers. A strong motivation for scaling down resonators is to increase their sensitivity and reduce the effect of thermomechanical noise, thereby improving the resolution of resonant sensors and also enhancing their response time. This development has increased the sensitivity limit up to the extent that researchers can now visualize the counting of molecules. With the ability of high throughput analysis of analytes and ultrasensitive detection, NEMS resonators potentially hold tremendous promise for the next generation of miniaturized and highly sensitive sensors.

However, scaling the dimensions of a resonator down to the NEMS range, the only action of cantilever detecting cans highly perturb the system itself.

Optical detection is a well known method commonly used in detecting resonance frequencies in atomic force microscopes and in mass/force sensing. The method focuses a laser spot on the surface of cantilevers to be measured, offering the possibility to inspect all the dynamical properties of the beam.

In this work it is shown that thermal laser-induced effects can cause a significant amount of frequency shift in the resonator. FEM simulations reveal the importance of the effect of the thermal-induced surface stress on the frequency resonance shift. Thermal laser-induced stresses strongly modify the dynamical properties of ultrathin cantilevers, affecting in a drastic way their measurement accuracy. Our theoretical work suggests that laser detection effects have to be seriously take into account when resonator dimensions are strongly reduced.

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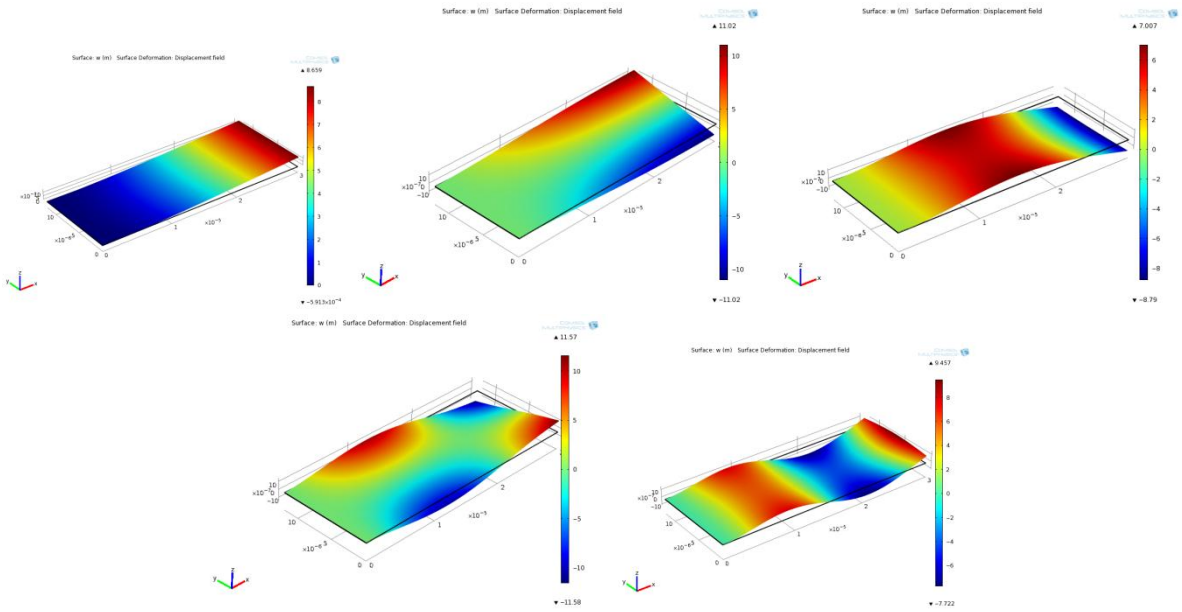

Fig.1 FEM simulation of the first five resonance mode of an ultrathin cantilever (50 nm) subjected to a no-linear deformation produced by thermal-induced surface stresses.

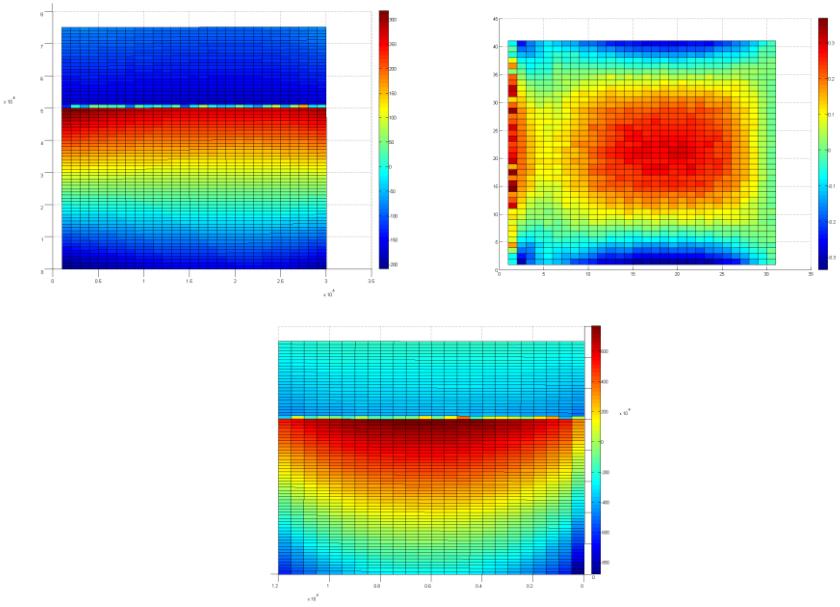

Fig.2 FEM simulations of the thermal-induced axial stress σ_x integrated along the X, Y, Z axis.

Low and High resolution Parallel Software for HAADF-STEM Image Simulation

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High Angle Annular Dark Field Scanning Transmission Electron Microscopy (HAADF-STEM), also known as Z-contrast is obtained by scanning an electron probe of atomic dimensions across the specimen and collecting electrons scattered to high angles. HAADF images are relatively immune to defocus and/or thickness effects contrary to an image obtained with a conventional transmission electron microscope (CTEM). They are also more sensitive to elements with large atomic numbers than those with small Z's providing chemical information at the nanoscale. A widely used methodology for precise atomic structural and composition analysis consists on comparing simulated images to experimental observations. This makes necessary the use of powerful image simulation tools for the research and study of nanostructures.

SICSTEM[1] is a parallel software code developed for running on the University of Cadiz Supercomputer (3.75 Tflops) that allows the simulation of high resolution images from large nanostructures containing more than one million atoms in reasonable time (from hours to a few days). The software has been designed to be able to generate not only one dimensional line scans or two dimensional images, but also to perform optical sectioning in the STEM simulation process. The input to SICSTEM software is a supercell described as a set of <x, y, z> coordinates for atom positioning, its composition, site occupancy, and Debye–Waller factor and the characteristics of the microscope: beam energy, third and fifth order objective aberrations, objective aperture, detector angles, etc. The image is simulated following a multislice[2,3] schema. We illustrate the results obtained by applying SICSTEM software to generate HAADF-STEM simulated image from an InAsP self-assembled nanowire. Specifically, an uncapped InAs quantum nanowire deposited by molecular beam epitaxy on an InP(001) substrate and periodically arranged along [110]. The z axis was defined as zone axis-crystal. The model was defined taking into account shape, compositions, boundary conditions and elastics parameters of the materials. The InP substrate was defined to be 8 nm high, the wetting layer 0.35 nm high and the wire was defined to be an isosceles triangle with two equal angles of 19,47º a side of 12 nm and 2.10 nm high. Model size was defined to be 18x15x10.45. Fig.1 shows the model and mesh used and the simulated image. The overall simulation process was 32 hours for a 575x982 pixels resolution image.

LowRes_SICSTEM is a low resolution HAADF-STEM software[4,5] based on the FFT multislice. For simulation purposes, the specimen is represented by a 3D arrangement of cubes where each cube is described by its chemical compositions, atomic density and atomic numbers. The probe, distributed in a Gaussian way, is set to an specified position (x,y,z) on top of specimen and illuminates the surface of several elementary volumes of the specimen which are inside the probe. The total intensity diffused at slice z is calculated as the weighted sum of all the n elementary cubes bombarded by electronic probe. This process is repeated slice by slice and the total intensity is computed by summing up contributions from all slices which determine the pixel intensity at each position in the image. The software has been

implemented using the Jacket platform for CUDA programming[6]. CUDA is NVIDIA's parallel computing architecture and enables a significant increase in computing performance by exploiting the power of the GPU (graphics processing unit). For tomographic reconstruction purposes the software is able to generate 2D projections from the model at any desired angle. The results of applying this software to generate simulated images from 3D model of Cu and Ag precipitate on cubic geometry shape laying on a substrate of C is shown in figure 2.

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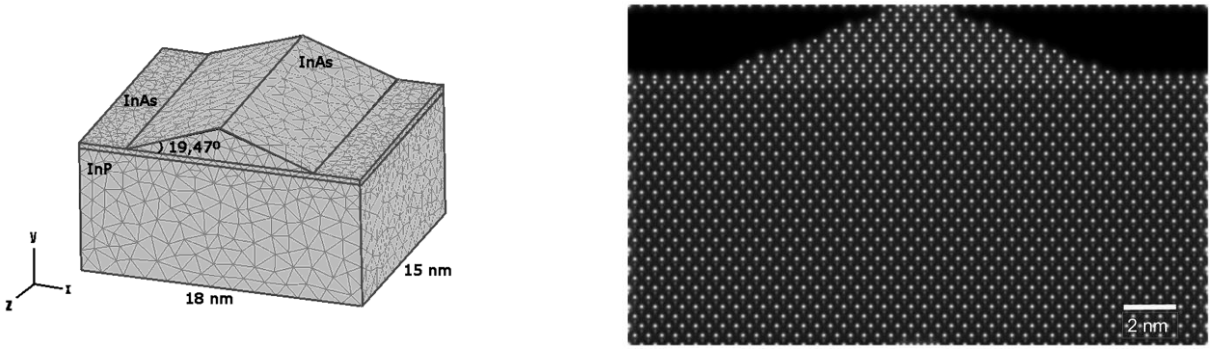

Figure 1: 3D InAs nanowire on InP sustrate model and simulated image.

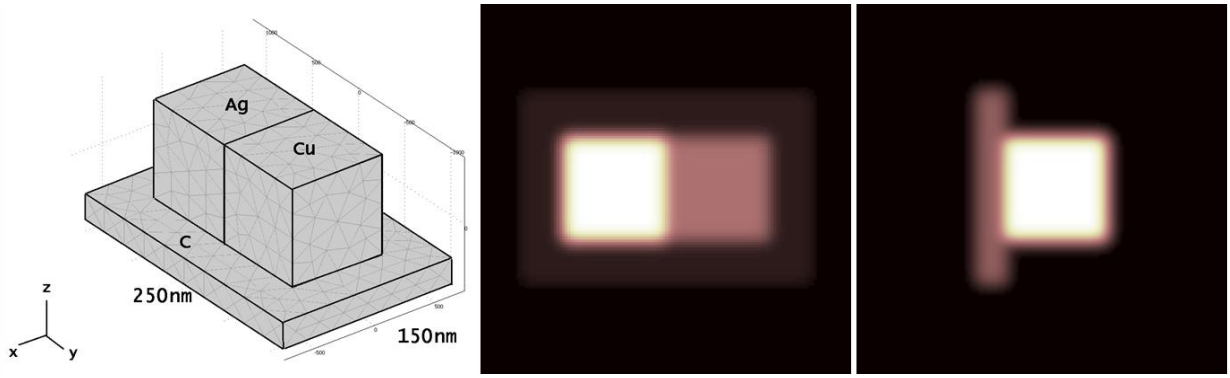

Figure 2: 3D model of Cu and Ag laying on a substrate of C and simulated images at two different projections (0 and 90 degrees around x-axis)

3D Electron Tomography in GPGPU

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3D Electron Tomography (ET) is concerned with the reconstruction of 3D volumes using a set 2D images obtained in the electron microscope. ET images suffer geometrical distortions introduced by the electrical and mechanical noise of real devices. Moreover, the effect of the scattering affect the quality of the reconstructed volume. The reconstruction process include the alignment of the series, that is the correction, of the geometrical distortions. These kind of correction can be based on image processing and features extracting techniques. Due to the huge dimension of the tomography data, parallel computing is a necessary tool in order to obtain good reconstruction in short times.

A tomography software prototype capable of performing a whole reconstruction process (alignment and volume recovering) of a full resolution volume (1024 x 1024 x 1024 voxels) starting from experimental images obtained in STEM mode has been developed. The prototype implements a semi – automatic alignment method designed for needle – shaped specimens for which classical alignment methods doesn't work in an optimal way. The tomography series supplied to the system is filtered in order to put in evidence those regions of the images in which the object of study lies, thus allowing the selection of these region that can be used as markers to align the series. The reconstructed volume of a needle – shaped specimen containing quantum dots (QDs) is shown as a result of the reconstruction process.

In our method, we consider single axis mode, thus allowing a per – slice approach to reconstruct the volume. Indeed, the aligned series has been considered a stack of 2D tomographies having the same 2D weight matrix. Simultaneous Iterative Reconstruction Technique (SIRT) has been chosen as reconstruction method because of its robustness to noise. The software has been deployed using MATLAB R2009A for the alignment and Compute Unified Device Architecture (CUDA) for the reconstruction. CUDA is the General Purpose Graphic Processing Unit (GPGPU) framework developed by NVIDIA that supplies high – level programming environment to use GPGPU capabilities. The implementation of SIRT on GPGPU allows a drastic reduction of the time needed to process a slice. Therefore, the entire volume can be reconstructed at its full resolution in less than 2.5 hours.

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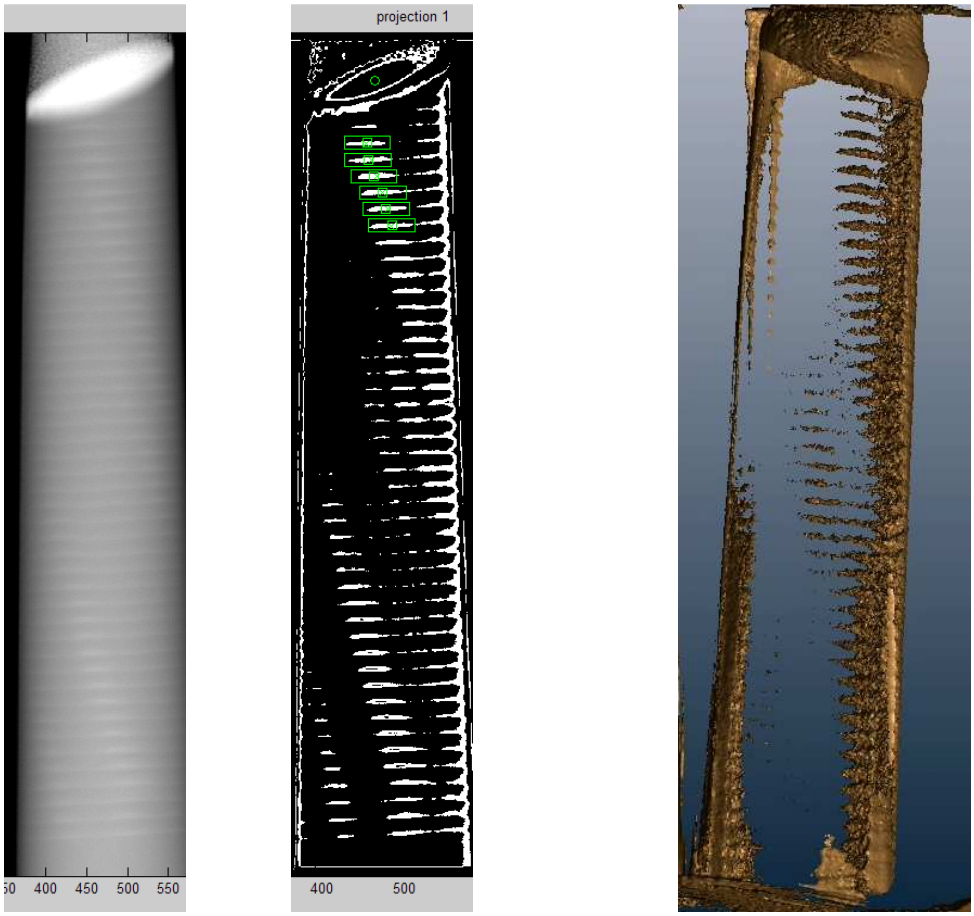
Figures



(a) (b) (c)

Figure 1: (a) Needle – shaped specimen, (b) segmentation and markers selection, (c) reconstructed volume.

Theoretical study of band alignment in nano-porous ZnO interacting with substituted Phthalocyanines

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The aim of this work is the theoretical study of the band alignment between the two components of a hybrid organic-inorganic solar-cell. The working organic molecules are metal tetra-sulphonated phthalocyanines (M-Pc) and the inorganic material is nano-porous ZnO growth in the 001 direction.

The theoretical calculations are being made using the density functional theory (DFT) using a GGA functional with the SIESTA code, which projects electron wave functions and density onto a real space grid and uses as basis set a linear combination of numerical, finite-range localized atomic orbitals. We also used the DFT+U method included in the code that allows a semi-empirical inclusion of electronic correlations in the description of electronic spectra for systems such as zinc oxide.

Basis set were optimized in order to obtain good ground state energies, cell parameters and bond lengths in bulk ZnO. Furthermore C and N basis set were optimized to minimize the energy in the Pc. First the ZnO and the M-Pc's have been studied individually.

For the M-Pc's we study the more stable geometry and the HOMO and LUMO for different metals (Zn and Cu) finding the most reacting part. The molecule is flat except the sulphonic groups which can freely rotate. The effect of these groups on the interaction with the nanostructure appeared to be very important for the bonding and not only for the molecule solubility.

Different ZnO surfaces have been modeled to find the optimal configuration, in their most stable wurtzite phase, and relaxed to find the minimum energy positions. The (001) growth direction was studied, so the available faces to the dyes will be a perpendicular one as the (100).

After that we study the interaction between the two systems and compared the different electronic energy levels. Different parallel and perpendicular orientations have been tested. We have obtained the total and projected density of states of the system and observed the level alignment. The aim was to determine which metal would be theoretically more efficient in the charge transfer between the dye and the nanostructure. A good estimation of band alignments between the adsorbate and the substrate was achieved with DFT+U, using the correlation corrections that gave good spectra for both systems separately. This theoretical study can be seen as a first step to show how charge transfer would be.

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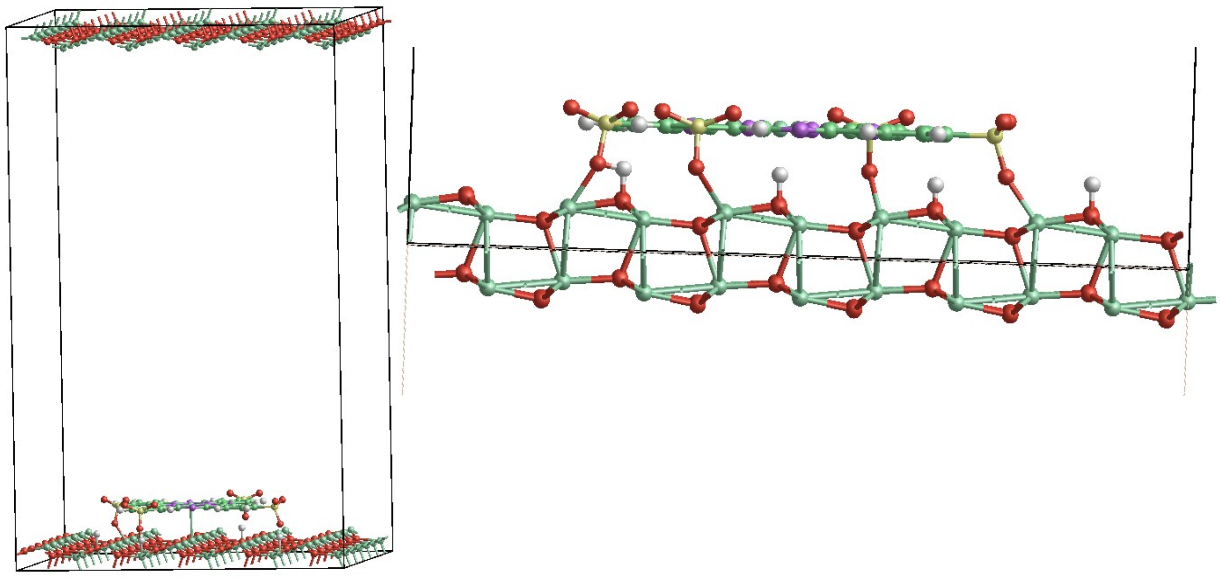
Figures



The most stable orientation we expect between the dye and the nano-structure.