### Microsymposia

In the framework of this approach, results of recent studies of local atomic and electronic structure for several types of nanostructures: free and supported Cu nanoclusters, magnetic nanoclusters, and irradiated by C and Si ions ZnO thin films are reported. The parameters of local atomic structure obtained from the XANES spectra analysis have been controlled by using theoretical optimization of the atomic structures on the basis of density function theory. The research is supported by RFBR 10-02-92658-IND\_a and the President of Russian Federation MK-4283.2010.2 grants.

[1] Grigory Smolentsev, Alexander V. Soldatov *Computational Materials Science* **2007**, *39*, 569.

**Keywords: XANES** 

### MS.56.3

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Graphene, electrons, plasmons, and quantum: A perfect match F. Javier Gacía de Abajo, Instituto de Óptica-CSIC, Serrano 121, 28006 Madrid, (Spain). E-mail: J.G.deAbajo@csic.es

Electron beams constitute excellent tools to probe both propagating and localized plasmons with outstanding spatial resolution. The inelastic events recorded in electron energy-loss spectroscopy (EELS) and in light emission during electron-plasmon interaction (cathodolumisnescence, CL) have been recently used to resolve plasmon excitations and to yield maps with detailed spatial distributions [1]. Here, we will illustrate several recent examples of plasmon mapping via EELS and CL in both extended metallic nanostructures and in nanoparticles. We will also discuss plasmons in graphene as an emerging powerful framework to study the interaction between photon, plasmons, and electrons at the single particle level, with potential applications to areas as varied as ultrasensitive biosensing, nonlinear optics, and quantum information processing.

[1] F.J. García de Abajo, Reviews of Modern Physics 2010, 82, 209-275.

Keywords: plasmon, EELS, cathodoluminescence

### MS.56.4

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# Amphipathic and amphidynamic crystalline materials: an XRD and MAS NMR study

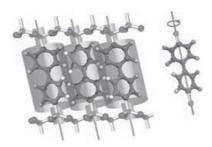
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Molecular self-assembled crystalline materials are promising in several fields, including gas storage, selective recognition and modulation of functions of active molecules. The tandem X-ray diffraction and solid state NMR approach allowed us to study amphipathic or amphidynamic materials i.e. crystalline structures that exhibit an intrinsic duality within the same periodic architecture [1-4]. In particular, we realized self-assembled crystalline architectures with guest molecules compartimentalized in two amphipathic nanospaces with distinct geometries and polarities [5]. The effect of these distinct environments on the NMR properties of the guest molecules is evident from chemical shift data and 2D heterocorrelated NMR techniques that could discriminate identical guest molecules embedded in distinct structural environments - one highly polar and the other nonpolar. The large magnetic susceptibility effect, due to ring currents of the

aromatic host, enabled the determination of the host-guest distances and corroborated the variable-temperature crystal structure resolution. A dual behavior was also highlighted in a block copolymer. The molecular recognition of specific blocks of triblock copolymers by a host molecule led to the formation of hierarchical periodic structures [2]. The end blocks of the triblock copolymer were locked into the inclusion crystals whilst the central block was excluded, creating a new material of assembled nanocrystals regularly superimposed on one another. The formation of the supramolecular architectures was followed *in situ* synchrotron X-ray diffraction while fast-¹H MAS NMR provided direct evidence of selective inclusion of the blocks.

Notably, amphidynamic materials could be recognized in hybrid organic-inorganic crystalline materials [1]. The precise engineering of highly-organized porous materials containing organic elements pivoted on inorganic layers enabled the fabrication of fast molecular rotors entirely exposed to the guest molecules exploring the cavities. Powder X-ray diffraction highlighted the crystalline order on both the meso- and molecular scales. Spin-echo deuterium NMR gave direct proof of the reorientation rate of the aligned rotors and demonstrated the active role of the guests in modulating the rotor dynamics.

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Keywords: NMR, inclusion, dynamics

#### MS.56.5

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## Metal-semiconductor surface phase transitions: A photoelectron – diffraction study

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The origin of surface phase transitions has been a matter of intense dispute among theoreticians and experimentalists, during the last years. Concurrently, inside surface science, systematic studies of simple model systems has successfully provided remarkable advances during the last 40 years. In spite of this, the emergence of novel powerful techniques has made attainable a more truthful representation of those "well-known" traditional systems. The improved new pictures confirm that complex phenomena take place at surface originally described as simple model systems. In particular, notions as Peierls distortions, Fermi surface nesting, Jahn-Teller distortions, metalinsulator fluctuations, disproportionation and charge and spin density waves, have been pointed out as responsible mechanisms of reported Surface Phase Transitions. In this sense, pioneer studies have focused their attention on the traditional Pb or Sn adsorbed on Ge(111) surfaces,