Several approaches have been made to deal with this issue. One classical teaching pamphlet is that produced by Elizabeth A. Wood, 1972 [1] which was translated to most of the most popular languages. More recently this subject has been discussed in several papers by Kantardjieff [2]. Concerning Spain, some successful attempts have been developed to make crystallography and crystallization close to students. One of these is the so call Crystallization in the School [3]. This crystal growing competition has been organized since 2008 involving several high schools within the region of Andalusia (Spain), Puerto Rico, Asturias and, during the present academic year, it has been extended throughout the whole of Spain.

Within the Spanish initiative for excellence (CEI), the Summer Scientific Campus offered by the University of Oviedo -CEI has the aim of promoting the scientific vocations amongst near-future graduate students who are immersed during 14 days on different profiles of experimental sciences, technologies and innovation within a unique environment of cultural exchange, with the experimental science activity, through their integration into research projects carried out in the university facilities.

We have developed a proper scenario to incorporate Crystallography into the Summer Scientific Campus, presenting the X Ray Diffraction topics in a substantive way and trying to attract the enthusiasm of youngest into Crystallography, using the Forensic Science as an appropriate setup to understand the techniques and authentic processes used within a Crime Scene. Our 'X-Ray diffraction in the Forensic Science Workshop' introduces and develops the skills, understanding and knowledge of X Ray diffraction methods and their application to forensic science.

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**Keywords: teaching crystallography, forensic science, summer scientific school**

## MS98.P01

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### Structural basis for the mechanical deformation in organic solids

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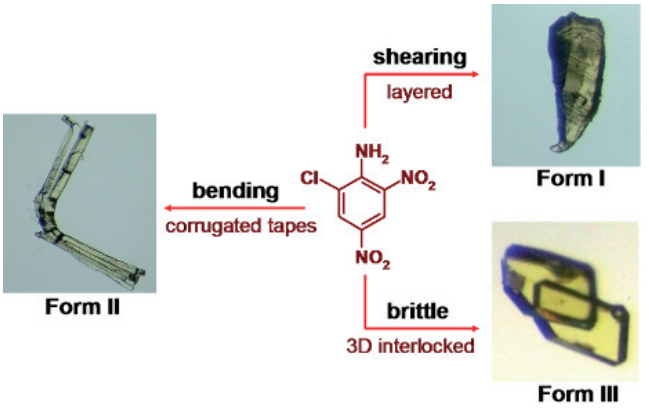
Understanding structure-mechanical property correlations is a key element in material science and engineering that underlies the successful design of materials [1], [2], [3], [4]. Based on mechanical behaviour, molecular crystals may be classified into three categories: (1) shearing, (2) bending and (3) brittle [5]. Crystals with parallel layered structure having strong intralayer and weak interlayer interactions show shearing on application of a mechanical stress. Bending occurs when the strength of intermolecular interactions in orthogonal directions are significantly different. Isotropic crystals with comparable intermolecular interactions in the three orthogonal directions display brittle nature. The experimental characterization of the defects or molecular packing at the deformed region is challenging as the organic materials are generally very sensitive to the microscopy beams.

In our ongoing study, the mechanism of crystal deformation is being investigated by probing the deformed region using a combination of techniques like, single crystal X-ray structure determination, micro Raman, HRTEM and optical microscopy. The preliminary results on bending type crystals suggest that the ordering of molecules at the deformed region is not completely random as in amorphous materials, but the deformed region turns into the polycrystalline domains with slightly altered molecular packing. It was also observed that the severe bending in the crystals leads to the formation of grain boundaries within which the molecules adopt somewhat distinct (high energy) packing.

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**Keywords: mechanical, deformation, bending**

## MS98.P02

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### Highly symmetric complex intermetallics

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A growing number of structurally highly complex intermetallic phases is being discovered and described with the emergence of new crystallographic methods. We are still not able to understand, why unit cells containing hundreds or even thousands of atoms are being formed by simple, binary and ternary metallic compounds. To approach this important question we are working on a systematization of complex intermetallics, starting with the highest-symmetric lattice, *i.e.* the cubic face-centered structures.

There is a bigger group of phases with approximately 400 atoms per unit cell - 43 reported structures -, which crystallizes in only two different space groups and can be roughly assigned to a common aristotype structure. The few structures with even bigger unit cells - 11 phases with around 1000 atoms per unit cell, not mentioning the even bigger Al-Cu-Ta compounds [1] ,[2] - show a slightly broader structural variety but can also largely be traced back to some common geometrical characteristics. We try to understand all of these structures in terms of the cluster approach, describing them as packings or coverings of highly symmetric building blocks. In addition, features of the average structure and findings from first-principle studies are

discussed with respect to complexity and phase formation.

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**Keywords: intermetallic, cluster, superstructure**

## MS98.P03

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**Unusual orbital and atomic ordering in tetragonal phase of $MgTi_2O_4$**

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It is theoretically shown that the structure of the tetragonal phase $MgTi_2O_4$ contains metal pico-and nanoclusters: two types of dimers $Ti_2$, two types of helices along the axis of the second and fourth-order of tetragonal cell and two types of one-dimensional infinite strands of titanium ions. Such unusual structural features of magnesium titanite arise due to atomic and d-orbital ordering.

A theory of structural phase transition in $MgTi_2O_4$ is presented: the symmetry of the order parameter, thermodynamics and mechanisms of formation of atomic and orbital structure of the low-symmetry phase $MgTi_2O_4$ are studied. The critical order parameter, which induces a phase transition, has been stated; it is shown that the calculated structure of the tetragonal phase $MgTi_2O_4$ is formed as a result of the displacements of magnesium, titanium and oxygen, the ordering of oxygen atoms, ordering $d_{xy}$, $d_{xz}$, $d_{yz}$ – orbitals. It is proved that the contribution of non-critical representation in the ions displacements is insignificant.

In the framework of the sixth degree of the components of the order parameter of the Landau theory the possible phase diagram is constructed and it is shown that the changes of phase states can be carried out as a result of phase transitions of second and first order: high-symmetry phase borders with two low-symmetry phases along the lines of transitions of second order, and the border between low-symmetry phases is the line of the phase transitions of first order.

The proposed theory is in accordance with experimental results [1].

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**Keywords: Spinel, Orbital, Ordering**

## MS98.P04

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**Self-assembly of nanoparticles into planar modulated superstructures**

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The advance in the synthesis of nanoparticles and colloids opens up the possibility to use them as building blocks for self-assembling novel materials. Ordered structures are especially interesting because they have unique photonic and electronic properties. Among the most complex ordered phases are commensurately and incommensurately modulated crystals. Although frequently found on the atomic scale in the bulk and as ordered structures of noble gases in adsorbed layers, modulated phases have so far not been known to self-assemble with nanoparticles.

Here, we use computer simulations to study a two-dimensional system characterized by a simple isotropic interaction that could be realized in future with building blocks on the nanoscale. We find that the particles arrange themselves into planar hexagonal superstructures whose superlattice vector can be tuned reversibly by changing the temperature. Thermodynamic stability is confirmed by calculating the free energy with a combination of thermodynamic integration and the Frenkel-Ladd method. Different contributions to the free energy difference are discussed.

[1] M. Engel, *Phys. Rev. Lett.* **2011,** *106*, 095504.

**Keywords: quasicrystal, modulated, 2D**

## MS98.P05

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**Crystal structures of new superconducting compounds, $LnT_2Zn_{20}$ (*Ln* = La, Pr, *T* = Ru, Ir)**

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In recent years, the cluster compounds and/or the compounds having cage-like substructure have attracted much attention not only in chemistry field but also in field of solid-state physics, to show rich interesting properties, since the discovery of fullerenes and fullerides. For example, in solid-state field, these compounds (especially, having rattled atoms in the cluster/cage structure) show various kinds of physical properties such as strong electron-phonon coupling superconductivity [1], heavy fermion behaviour [2], and thermoelectricity with glass-like thermal conductivity [3].

Last year, we found new superconducting compounds; $LnT_2Zn_{20}$ (*Ln* = La, Pr, *T* = Ru, Ir), showing superconducting transitions at *Tc* around 0.2 K ($LaRu_2Zn_{20}$), 0.6 K ($LaIr_2Zn_{20}$), and 0.05 K ($PrIr_2Zn_{20}$). Especially, $PrIr_2Zn_{20}$ is the second example of superconductor in the intermetallic compounds containing Pr atom. [4] Before taking superconducting state, these compounds take structural transitions, but do not have any magnetic transitions. At room temperature, the crystal structure of these compounds basically takes cubic $CeCr_2Al_{20}$-type structure (Fd-3m). [5] Details of the crystal structure are not so clear.

To understand the detail of this crystal structure, we carried out single-crystal diffraction technique at 293 K. Our used single crystals are grown by Zn self-flax method. [6] In the structure, *Ln* atom locates in the cage structure formed by 16 Zn atoms. On the other hand, *T* atom is surrounded by 12 Zn atoms forming another cage structure. Both *Ln* and *T* atoms locate at crystallographically independent sites. However, some of Zn sites show the site disordering behaviour. More details will be presented.

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