

it is evidenced that the second layer molecules are found to adsorb directly on top of the underlying layer.

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## MS63.P24

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### Structure solution of decagonal ZnMgDy quasicrystal

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Here we report the first structure solution of decagonal ZnMgDy quasicrystal (d-ZnMgDy) based on single crystal X-ray diffraction data. Samples with the composition ( $\text{Zn}_{57.6}\text{Mg}_{40.8}\text{Dy}_{1.6}$ ) were prepared by induction melting followed by annealing at 375°C for 10 months. The alloys were then quenched to room temperature. The resulting samples consist mainly of a hexagonal phase with the d-ZnMgDy existing as the secondary phase. The morphology of the decagonal phase is typically needle-like. These grains are of 50  $\mu\text{m}$  in length and approximately 15  $\mu\text{m}$  in other dimensions. X-ray diffraction experiments were carried out both in-house (Oxford Xcalibur PX diffractometer, CCD detector, Mo K $\alpha$  radiation) and at the Synchrotron facility in Swiss-Norwegian beam line, ESRF, Grenoble ( $\lambda=0.6980$  Å).

The Laue group was specified to be 10/mmm with a periodicity of 5.22 Å along the periodic direction. No systematic extinctions were observed. SUPERFLIP program package [1] (based on charge flipping and low density elimination algorithms) was used for structure solution.

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**Keywords:** quasicrystal, decagonal

## MS63.P25

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### Analysis of structure and chemical order in a ternary Yb<sub>12</sub>Mg<sub>52</sub>Cd<sub>36</sub> quasicrystal

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The atomic structure of the ternary Yb<sub>12</sub>Mg<sub>52</sub>Cd<sub>36</sub> quasicrystal has been refined from single crystal X-ray data. The ternary quasicrystal is related to the binary i-Yb<sub>16</sub>Cd<sub>84</sub> parent phase, [1, 2] and suffers from chemical disorder mainly due to mixing between Mg and Cd. Studies on related ternary approximants however indicate that this chemical disorder is only partial, and that there are strong selection rules in

several ternary systems that govern the choice of a particular atom at a specific site. The purpose of this work is thus to elucidate the chemical order between the constituent elements in the ternary Yb<sub>12</sub>Mg<sub>52</sub>Cd<sub>36</sub> quasicrystal and its relation to ternary approximants in other RE-Mg-Cd (RE=Rare Earth) systems. The structure refinements performed on the Yb<sub>12</sub>Mg<sub>52</sub>Cd<sub>36</sub> quasicrystal clearly indicate that it is composed of similar atomic clusters as the binary i-Yb<sub>16</sub>Cd<sub>84</sub> phase and that there is a strong selection rule that mainly determines the chemical order at the cluster level. Similar observations have also been made in other related ternary approximant phases. The structure refinement is the first of its kind performed on a ternary Yb-Cd-related quasicrystal, and the results indicate that the structures and chemical order of ternary quasicrystals can be understood by extracting and combining information from structure refinements on both quasicrystals and related approximants.

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**Keywords:** quasicrystal, approximant, chemical order

## MS63.P26

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### Ab-initio calculations on the stability of heptagonal ordering in Gallium

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Sevenfold symmetry is the lowest rotational symmetry not yet observed in quasicrystals. However, there are several strong hints that indicate the existence of heptagonal quasicrystals (QCs) [1]. In a previous ab-initio study [2] it was shown that theoretical sevenfold approximants, designed from promising known boride and borocarbide structure types by using a supertile approach, were acceptably stable within the range of error. Due to the fact that these structures and their associated tilings are ternary, the weak matching rules automatically imposed on the edges of the tiles only allow for a limited number of possible structural arrangements.

The configurational degrees of freedom can be increased by investigating the structure of monatomic  $\gamma$ -Ga, a metastable low temperature phase that forms when undercooling liquid Ga to below -35.6 °C. Its structure consists of regular sevenfold antiprisms centered by a single Ga atom. Additionally it can be described as a periodic arrangement of one of the three heptagonal rhombic unit tiles, namely the "fat" tile with an ideal acute angle of  $3\pi/7$  ( $= 77.12^\circ$ , in the structure  $76.15^\circ$ ).

For the missing two unit tiles (with acute angles  $\pi/7$  and  $2\pi/7$ ), decorations were designed by using similar atomic arrangements as for the fat tile (i.e.  $\gamma$ -Ga). As only periodic structures can be accessed by means of ab-initio total energy calculations, the unit tiles were subsequently used to decorate approximants. Therefore various theoretical structure types were generated, either by periodic arrangement of single tiles or hexagon supertiles of the rhomb tiles, or by creating rational heptagonal approximants using the cut-and-project method.

The first-principles DFT calculations were performed with the VASP code [3], using a plane-wave basis set, the GGA algorithm and PAW-PBE pseudopotentials. Total energies were calculated for all theoretical Ga structure types, as well as the electron localization function (ELF), and the atom relaxation movements were investigated.

The possibility of stabilizing the designed structures by dopant atoms was also explored: the rational approximant structures mentioned above exhibit a small number of voids or holes too large for Ga-atoms,

which were filled with other atoms from the boron group (In and Tl) by 3 to 5 at.%. The binary convex hulls for these systems were also calculated.

From our results we compare the mechanical and energetical stability of different types of theoretical heptagonal approximants, in relation to the stable modifications of Gallium. We could draw conclusions about the mechanisms of heptagonal ordering in Gallium from the structure types decomposing during relaxation. We were also able to estimate the influence of doping on the stability of our approximants.

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**Keywords:** gallium, quasicrystal, calculation

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### A novel structure: PSPC1/NONO heterodimer, members of the DBHS protein family

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Proteins of the Drosophila Behavior and Human Splicing (DBHS) family share a common domain structure: two RNA recognition motifs (RRMs), a NONA/Paraspeckle (NOPS) domain followed by a coiled-coil region. Paraspeckle Protein Component 1 (PSPC1) and Non-POU domain-containing octamer-binding protein (NONO) are members of this family and have a highly similar sequences within the DBHS domain. PSPC1 and NONO form a heterodimer and they are co-localised to paraspeckles, a dynamic sub-ribonuclear bodies in eukaryotic cells [1]. These proteins will be recruited to paraspeckles at the point of transcription of a long non-coding RNA, called NEAT1 which forms the structural scaffold of these bodies [2,3,4]. Within paraspeckles, PSPC1 and NONO are involved in transcriptional regulation by confining RNA to the nucleus, preventing subsequent protein production [2,3,4]. However, the mechanisms at the molecular level behind these processes are still unclear. Structural analysis of PSPC1 and NONO and investigation of RNA binding partners will broaden the knowledge about their functions in transcriptional control. Here we present the first paraspeckle protein structure, the PSPC1/NONO heterodimer. This structure highlights the DBHS domain with a novel arrangement of four different RRM. Furthermore, we describe a new protein-protein interaction domain (NOPS). We also observe the first example of an anti-parallel right handed heterodimeric coiled-coil. This PSPC1/NONO structure provides us with new insights into the functions of paraspeckle assembly as well as possible RNA binding modes.

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**Keywords:** paraspeckle proteins, rna-recognition motif, coiled-coil

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### Structural basis of inhibition mechanism by carrot EDGP against endoglucanase

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Plant cell wall is composed of various polysaccharides such as cellulose, hemicellulose and pectin. Cellulose microfibrils are linked via hemicellulose. The network of cellulose-hemicellulose provides tensile strength. Carrot extracellular dermal glycoprotein (EDGP) is one of proteinous inhibitor to protect cell wall. To penetrate and use plant cell walls nutritionally, pathogen secretes cell wall degrading enzymes. These enzymes including endoglucanases, xylanase and polygalacturonases are classified into glycoside hydrolase (GH) families. EDGP shows inhibitory activity against xyloglucan specific endo- $\beta$ -1,4-glucanase (XEG) from *Aspergillus aculeatus*. XEG belongs to GH12 family. XEG specifically cleaves xyloglucan that is a major hemicellulose of dicots. Xyloglucan consists of  $\beta$ -linked glucose backbone substituted with xylose side-chains. The degradation of xyloglucan is great damage for dicotyledonous plants. Thus, inhibition of XEG by EDGP is important in plant defense system. Until now, the homologous proteins of EDGP were found in various plants. The tomato homolog (xyloglucan specific endo- $\beta$ -1,4-glucanase inhibitor protein, XEGIP) and tobacco homolog (Necturin IV, NEC4) also inhibit XEG. In contrast, the homologous protein from wheat (*Triticum aestivum* xylanase inhibitor, TAXI) inhibits GH11 xylanases. Interestingly, a soybean homolog (Basic 7S globulin, Bg7S) lacks inhibitory activity for both GH11 and GH12 enzymes.

To clarify the inhibition mechanism of EDGP against GH12 endoglucanase, we work on structure determination of EDGP and EDGP in complex with GH12 enzyme by X-ray crystallography. EDGP and the inhibition complex with FI-CMCase, which is GH12 endoglucanase from *Aspergillus aculeatus*, were successfully crystallized. Hexagonal crystal of EDGP belonged to space group  $P6_6$ , with unit cell parameters  $a = b = 130.4$ ,  $c = 44.5$  Å and  $\beta = 120^\circ$ . Monoclinic crystal of EDGP complex with FI-CMCase belonged to space group  $C2$  and unit cell parameters  $a = 169.5$ ,  $b = 143.0$ ,  $c = 63.0$  Å and  $\beta = 110.9^\circ$ . The crystal structure of EDGP was determined by SIRAS method using iodine derivative crystal, and the crystal structure of EDGP~FI-CMCase complex was determined by molecular replacement. The structure of EDGP~FI-CMCase complex reveals that Arg423 of EDGP intrudes into the active site of FI-CMCase. The arginine residue is conserved in homologous proteins that have inhibitory activity for GH12 enzymes. This work provides structural basis of inhibition mechanism by EDGP and its homologous proteins against GH12 enzymes.

**Keywords:** plant, inhibitor, structure

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### Architecture of the mediator head module

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