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

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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 ($Zn_{57.6}Mg_{40.8}Dy_{1.6}$) 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 μm in length and approximately 15 μm in other dimensions. X-ray diffraction experiments were carried out both in-house (Oxford Xcalibur PX diffractometer, CCD detector, Mo Kα radiation) and at the Synchrotron facility in Swiss-Norwegian beam line, ESRF, Grenoble (λ=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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Analysis of structure and chemical order in a ternary $Yb_{12}Mg_{52}Cd_{36}$ quasicrystal

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The atomic structure of the ternary $Yb_{12}Mg_{52}Cd_{36}$ quasicrystal has been refined from single crystal X-ray data. The ternary quasicrystal is related to the binary i-$Yb_{16}Cd_{84}$ 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 $Yb_{12}Mg_{52}Cd_{36}$ quasicrystal and its relation to ternary approximants in other *RE*-Mg-Cd (*RE*=Rare Earth) systems. The structure refinements performed on the $Yb_{12}Mg_{52}Cd_{36}$ quasicrystal clearly indicate that it is composed of similar atomic clusters as the binary i-$Yb_{16}Cd_{84}$ 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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MS63.P26

***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 configuarational degrees of freedom can be increased by investigating the structure of monatomic γ-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 3π/7 (= 77.12°, in the structure 76.15°).

For the missing two unit tiles (with acute angles π/7 and 2π/7), decorations were be designed by using similar atomic arrangements as for the fat tile (i.e. γ-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,