Cd_6R(R:rare earth elements) crystals are regarded as 1/1 approximants to the $Cd_{5.7}Yb$ icosahedral quasicrystal[1]. At 300K, they are *bcc* phases which are made of so-called Tsai-type clusters. A Tsai-type cluster is composed of four successive atomic shells of, from the center, Cd_{20} dodecahedron, R_{12} icosahedron, Cd_{30} icosidodecahedron and Cd_{60} rhombic triacontahedron. At the center of the cluster, there exists a disordered Cd_4 tetrahedron.

An occurrence of a structural phase transition has been observed in a number of the Cd_6R crystals, which is attributed to orientational ordering of the central Cd_4 tetrahedra, resulting in various types of superstructures below T_c. First, we will describe and classify the superstructures of Cd_6R and then discuss key factors which strongly influence the transitions based on the observations.

The Cd_6R crystals are also of interest in view of the magnetism since recently they are found to exhibit magnetic transitions below T_c in a striking contrast with the cases of other 1/1 approximants. For instance, three successive magnetic transitions have been reported for R=Tb[2] and Sm[3] with different magnetic orders at the lowest temperature, i.e., antiferro- and ferrimagnetic orders at 2K, respectively. We will present magnetic properties of Cd_6R(R=Nd, Sm, Gd, Tb, Dy) having the same C2/c-type superstructure below T_c and comparison of the magnetic orders in the isostructural compounds will be made.

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MS.63.2

A dense quasicrystalline phase of hard tetrahedra

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Quasicrystals have traditionally been discovered in many binary and ternary metallic alloys. It has now become evident that aperiodic order can also be found on larger length scales in soft matter with micelles, colloids and macromolecules [1]. The experimental findings that nanoparticles can self-assembly into highly complex, ordered structures are also backed up theoretically by computer simulations [2] which, due to the larger size of the particles involved and resulting simpler particle interactions, are well suited to reproduce and study the crystallization process.

As it is now possible to synthesize nanoparticles of various shapes and interactions with high yield and high structural perfection, these particles can be seen as building blocks for assembling novel materials from bottom up with the goal of improved or unusual electrical, mechanical or other physical properties. In my presentation I focus particularly on the behavior of hard regular tetrahedra. The tetrahedral shape is highly anisotropic and therefore in its behavior distinctly different from what is known from atoms and spherical colloids.

The question of how densely tetrahedra pack has attracted much interest over the last years. In a first study, we have reported the spontaneous formation of a dodecagonal quasicrystal in Monte Carlo computer simulations [3]. A crystalline approximant of the quasicrystal with an 82-particle unit cell was compressed to a then-record packing fraction of 85.03% [3]. Very shortly after, a family of dimers packings were proposed, which were subsequently optimized to a packing fraction of 85.63% [4], the currently densest known packing of tetrahedra.

Due to its higher packing density, the dimer crystal is thermodynamically favored in the limit of infinite pressure. However, which structure is stable at finite pressures is an open question. I will discuss how we use thermodynamic integration and free energy calculations to explore the relative stability of these very different ordered phases as a function of packing density [5].

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MS.63.3

Prediction of low-temperature phase transition in $Al_{11}Ir_4$ compound

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The average structure of the Al11Ir4 phase [1] exhibits mean occupancy of 0.5, providing 60 sites for 30 atoms in a cubic cell with 7.7A long side. To resolve the occupancy correlations, we employ ab-initio methods and empirical pair potentials fitted to ab-initio data. Our first result is that the part of the structure plagued by many nearby low--occupancy sites is an irregular $IrAl_{10}$ cluster. Due to mismatch between high (icosahedral) symmetry of the cage surrounding the low-symmetric $IrAl_{10}$ "core", the structure possesses configurational degrees of freedom down to low temperature. By simulated annealing in 4x4x4 supercell, we find phase transition at the temperature as low as 500 K. While the high-temperature phase has simple cubic symmetry (space group P23) in accordance with the experimentally refined structure, we predict the low-temperature phase is 2x1x1 supercell, with Pma2 space group. According to our ab-initio total energy calculations at T=0K, the low-temperature structure is stable against decomposition into competing crystalline phases.

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MS.63.4

The structure of Al-Cu-*Me* (*Me* =Co, Rh, Ir) quasicrystals

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We present a real space structure refinement of three decagonal phases: Al-Cu-Co, Al-Cu-Rh, Al-Cu-Ir. The structure factor, which

was used for the modelling process, was calculated using a statistical method [1], which allows a purely 3-dimensional, real space optimization of a quasicrystalline structure. Such an approach has already been successfully used for structure refinement of various modifications of the Al-Ni-Co quasicrystal [2], [3], [4]. This is the very first attempt of quantitative structure optimization of Al-Cu-Ir and Al-Cu-Rh quasicrystals based on high resolution, synchrotron diffraction datasets. Up to now the only structure investigation of an Al-Cu-Rh quasicrystal was based on electron microscopy, the structure of the Al-Cu-Ir quasicrystal has not been studied before and the Al-Cu-Co structure was refined only based on a rather limited, in-house diffraction dataset. The current refinement gives much more details about the structure.

All three decagonal phases show ~4 Å periodicity (two atomic layers per period). Their space group is centrosymmetric $P10_5/mmc$. While the Al-Cu-Co phase shows a significant amount of diffuse scattering in the interlayers of the diffraction pattern, the Al-Cu-Ir and Al-Cu-Rh phases exhibit no diffuse scattering. This fact is well-reflected in the structure of Al-Cu-Ir and Al-Cu-Rh phases, *i.e.* they are well-ordered, the Cu/Ir and Cu/Rh positions can clearly be distinguished and the only disorder present is the partial occupation of several Al positions. All decagonal quasicrystals are ternary alloys based on Al and two transition metals. This is the very first structure refinement of a decagonal phase distinguishing the positions of two different transition metal atoms. The initial model for all phases was the same and based on the rhombic Penrose tiling. The initial decoration of the rhombuses was derived based on a structure solution obtained from charge flipping. The refined structure gives reasonable R values, and the chemical composition agrees well with the EDX measurements.

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MS.63.5

Variable-Range-Hopping Conductivity in Quasicrystals

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Among icosahedral phases, including single crystals of icosahedral Al-Pd-Re, the variable-range-hopping (VRH) regime is only revealed in polygrain samples of icosahedral Al-Pd-Re with the resistivity ratio $R = \rho(4.2 \text{ K})/\rho(300 \text{ K}) \geq 13$. Experiments show that this regime relates to the presence of defects, voids and inclusions of secondary phases [1, 2]. Here we analyze the low temperature electronic transport in polygrain samples of icosahedral Al-Pd-Re using an analogy with granular electronic conductors. Our preliminary results are given in Ref. 3.

The density of electronic states at the Fermi energy $N(E_F)$ in icosahedral quasicrystals is nonzero. We therefore consider a model in which metallic quasicrystalline particles of a size ranging from few nanometers to hundreds of nanometers are embedded into an insulating matrix. The electronic levels are discrete due to electron confinement within a single "grain". The mean level spacing δ is inversely proportional to the volume V of the grain $\delta = 1/[N(E_F)V]$. For icosahedral Al-Pd-Re δ is an order of magnitude higher that for a typical metal.

Two main factors are responsible for the electronic transport in icosahedral Al-Pd-Re. The first is the dimensionless intergranular conductance g. Samples with $g \geq 1$ exhibit metallic properties. Samples with $g \leq 1$ show an insulating behavior. Depending on the structural state of the material and the temperature, both factors may be important. The notion of granular system means $g \leq g_0$, where g_0 is the dimensionless intragranular conductance. The homogeneously disordered case corresponds to $g \approx g_0$. The second factor is the electrostatic (Coulomb) energy $E_g \gg \delta$, which accounts for the change in the energy of a grain when an electron is added or removed. It plays an important role in the insulating regime when electrons are localized in the grains. At low coupling $g \ll 1$ an electron has to overcome an electrostatic barrier into a neighboring granule. Depending on the structural state and temperature the both factors may be important for the specific behavior of the electrical conductivity. The character of electrostatic disorder defines either the Efros–Shklovskii or the Mott type of the VRH regime primarily with elastic co-tunneling at $T \leq (\delta \cdot E_g)^{1/2}$. For icosahedral Al-Pd-Re this temperature is less than 10 K. For strong intergranular coupling, the metallic regime with a power-law temperature variation of the electrical conductivity σ takes place. At low temperatures the temperature-dependent part of σ is dominated by quantum-interference corrections.

The metallurgical reason for the specific behavior of polygrain icosahedral Al-Pd-Re most likely relates to the fact that the icosahedral phase is the primary crystallization phase only for alloys with rhenium content lower that 5 at.%. For icosahedral phase with 8.5 at.% rhenium the primary crystallization phase is Al_3Re that crystallizes in the shape of needles leading to porous ingots with numerous voids.

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MS.64.1

Structural basis for the sequential assembly of photosynthetic multienzyme complex

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Protein-protein interactions are likely to be generally important in coordinated regulation of metabolic pathways. In photosynthetic CO_2 assimilation pathway (the Calvin cycle), such regulation is partially achieved by an intrinsically disordered protein, CP12, which acts as a linker in the sequential assembly of Calvin cycle enzymes glyceraldehyde-3-phosphate dehydrogenese (GAPDH) and phosphoribulokinase (PRK). Both enzymes activities are inhibited when embedded within the GAPDH/CP12/PRK complex. The reversible association/dissociation of the complex are mediated by light/dark transitions, which are responsible for the changes in redox potential and the concentrations of metabolites such as NAD(H) and NADP(H). However, the molecular mechanisms for the sequential multiprotein assembly still remain elusive.

Here we report the crystal structures of GAPDH-CP12 complex and PRK from *Synechococcus elongatus* (Fig. 1). The structure of GAPDH-CP12 complex represents that the C-terminal region of CP12