Surfaces of quasicrystal approximants and related phases: structures & properties

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Because the typical length scale of their atomic structures can be large, caused by the combination of covalent and ionic interactions as well as the presence of conducting electrons, quasicrystals and related phases are rightfully considered to be the most complex compounds in the crystal chemistry of inorganic structures. This complexity extends to the surface, thus leading to unique surface properties – at least when compared to those of conventional alloys. Examples include the non-wetting behavior [1] and the catalytic activities and selectivities [2] of Al-based quasicrystalline approximants.

The surface properties of quasicrystal approximants and related phases are inherently tied to the peculiar atomic and electronic structures of the bulk crystals, which are best described by a stacking of highly symmetric polyhedra held by a network of bonds with a iono-covalent character. The detailed knowledge of the surface structures is a necessary prerequisite for further studies of surface properties. In this lecture, I will first show how methods based on the Density Functional Theory can help to determine surface structures, in combination with experimental measurements if applicable. I will then present a few examples to show how surface properties are controlled by their geometric and electronic structures [3,4].

References:

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