MS23 Quasicrystals and complex intermetallic materials

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From honeycomb structures to 2D quasicrystals: Alkaline earth metal decorated Ti_2O_3 monolayers

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Abstract

Honeycomb structures are two-dimensional networks with hexagonal symmetry. Most famous is the elemental honeycomb of graphene, but also binary honeycomb structures are well-known like h-BN, transition metal chalcogenides and binary oxides. Binary oxide honeycomb structures are characterized by six-membered rings formed from transition metal atoms, e.g. Ti or V, which are covalently linked via oxygen atoms. Expressed in a tiling decoration scheme, oxide honeycomb structures are represented by a unit cell containing two equilateral triangles, each decorated with one Ti atom in its centre and oxygen atoms at the centres of the sides as shown in Figure 1.

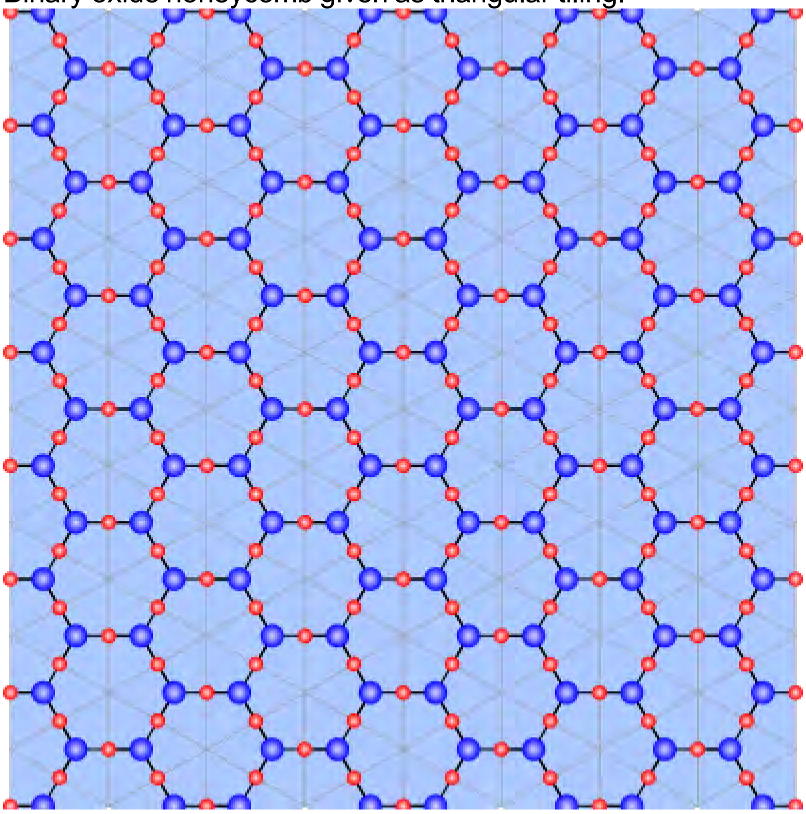
This talk bridges from binary oxide honeycomb structures to two-dimensional ternary oxide quasicrystals of dodecagonal symmetry that are formed from three tiling elements: equilateral triangles, squares and rhombuses [1]. The atomic structure of oxide quasicrystals has been under dispute in the past. By investigating a complex periodic quasicrystal approximant containing 48 triangles, 18 squares and 6 rhombuses (shown in Figure 2) we were able to decide between the competing structural models. Using scanning tunneling microscopy, surface X-ray diffraction and density functional theory calculations, we provide the experimental evidence that this extraordinary structure consists of an aperiodically ordered Ti_2O_3 network with rings of four, seven or ten Ti atoms (blue in Fig. 2) covalently linked via oxygens (red). These unfamiliar ring sizes are stabilized by the decoration with alkaline earth metal ions (green) [2]. The tiling decoration scheme derived from this model is able to explain the atomic structure of all experimentally observed periodic and aperiodic phases in two-dimensional ternary oxides and allows a classification of all structures according to their alkaline earth metal ion concentration[3].

Furthermore, we will show that an alkaline earth metal ion decorated honeycomb structure can be transformed into a dodecagonal oxide quasicrystal. This transition is accompanied with a workfunction change in the 2D oxide layer reporting on a change in the surface dipole induced by the alkaline earth metal ions in the two different geometries. The relation between honeycomb structures and dodecagonal oxide quasicrystals established here paves the way towards the exploration of new aperiodic two-dimensional oxide systems.

References

[1] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, Nature 502, 215 (2013).
[2] E. Cockayne, M. Mihalkovič, and C. L. Henley, Phys. Rev. B. 93, 026102 (2016).
[3] F. E. Wührl et al., Phys. Stat. Solidi B, 2100389 (2021).

Binary oxide honeycomb given as triangular tiling.



Unit cell of the 48:18:6 approximant in Sr-Ti-O.