Surface structures of several complex intermetallics with cluster-based bulk structures

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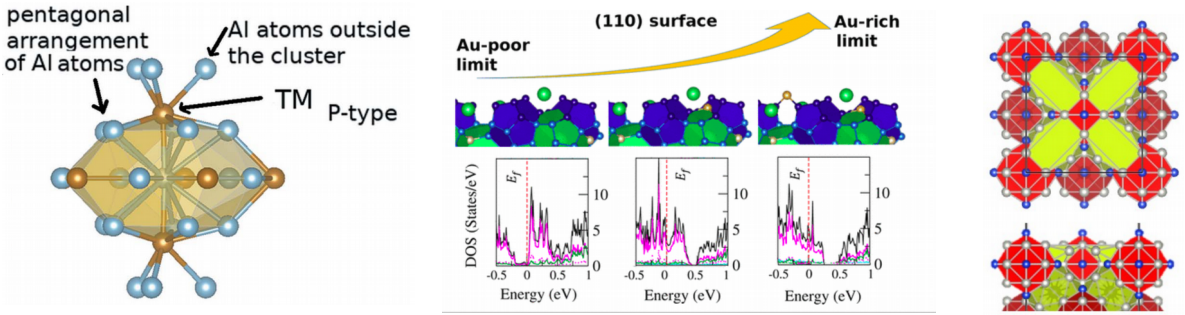
The bulk structures of most complex intermetallic compounds, like intermetallic clathrates, quasicrystals, their crystalline approximants and related phases, are described using building blocks based on polyhedral entities, often called "clusters". Typical clusters found in quasicrystals include the Mackay, Bergman and Tsai clusters, and numerous polyhedral shapes are used to describe complex intermetallics.
The structural complexity of these compounds extends to the surface. In this talk, the relationship between the three dimensional cluster-based bulk structure and the two-dimensional surface will be questioned, based on several examples including the pseudo-10fold surfaces of $Al_{13}TM_4$ (TM = Fe, Co) quasicrystalline approximants [1], the low-index surfaces of the $Ba_8Au_{5.25}Ge_{40.75}$ intermetallic clathrate [2] and the (100) surface of the $Ce_3Pd_{20}Si_6$ heavy fermion system [3], using a combination of experimental techniques under ultra-high vacuum and theoretical calculations based on the Density Functional Theory. The focus will be on the different mechanisms by which stable surface terminations are selected, to highlight the factors governing the atomic and electronic properties of the observed surfaces.



(a) (b) (c)

Fig. 1- (a) The Henley-type cluster found in the $Al_{13}TM_4$ quasicrystalline approximants. (b) Stable atomic and electronic structures for the $Ba_8Au_{5.25}Ge_{40.75}$(110) surface. (c) Top and side view of the $Ce_3Pd_{20}Si_6$(100) surface.

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[1] Ph. Scheid et al., Acta Cryst. A75 (2019) 314-324; É. Gaudry et al., Phys. Rev. B 94 (2016) 165406; J. Ledieu et al., Phys. Rev. Lett. 110 (2013) 076102
[2] K. Anand et al., J. Phys. Chem. C 122 (2018) 2215 and 29298.
[3] F. Abdel-Hamid et al., accepted, J. Phys. Chem. C (2019).