Complex energy landscapes of intermetallic compound surfaces for novel catalysts

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Because the typical length scale of their atomic structures can be large, quasicrystals and related intermetallic phases are rightfully considered to be among the most complex compounds in condensed matter. 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 and the catalytic performances of Al-based quasicrystalline approximants [1,2].

The surface structures and properties of complex intermetallic compounds 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. If crystal structures can be viewed as repositories of information, then crystal surfaces offer a pathway by which this information can be transferred to adlayers, molecular films or other two-dimensional systems that can be grown on them. Interestingly, quasicrystalline order can also emerge at the surface without being induced by a substrate of complex structure, as it is the case for the recently discovered quasicrystalline oxides [4].

In this talk, I will first show how methods based on the Density Functional Theory can help to determine surface structures [4], in combination with experimental measurements in most cases. I will then focus on the catalytic properties of selected complex intermetallic compounds [5,6], to show how they differ from the ones of simple alloys. Finally, I will discuss the influence of the surface electronic structure and morphology on the catalytic properties and propose a few perspectives of this work.

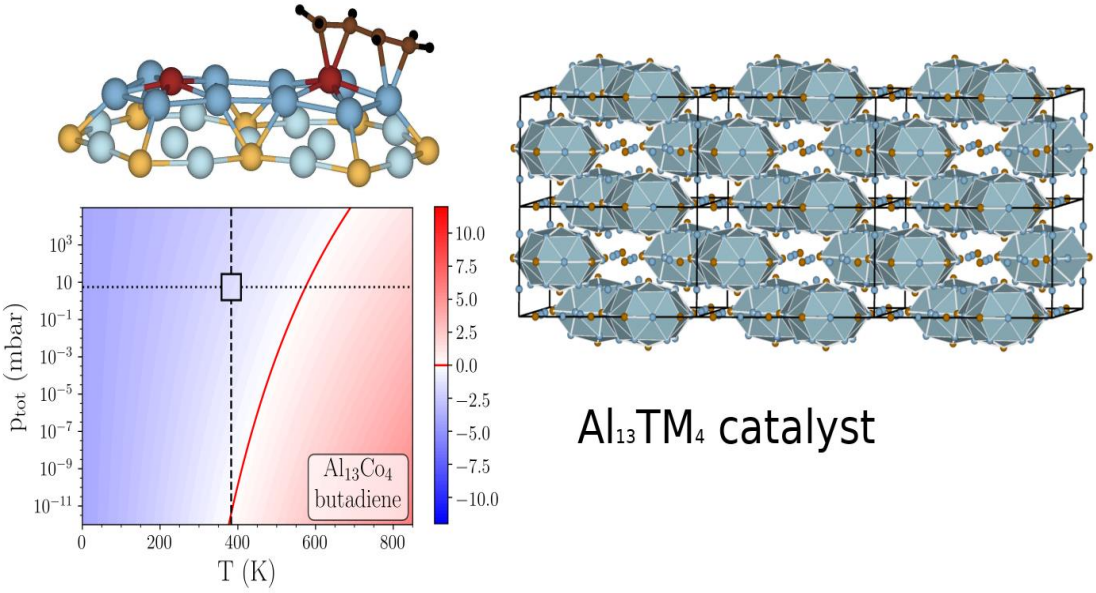

Figure: butadiene adsorption on the $Al_{13}Co_4(100)$ surface

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