Influence of the 3-dimensional cluster and preparation conditions on the structure of Al_5Co_2(210) and (100) surfaces.

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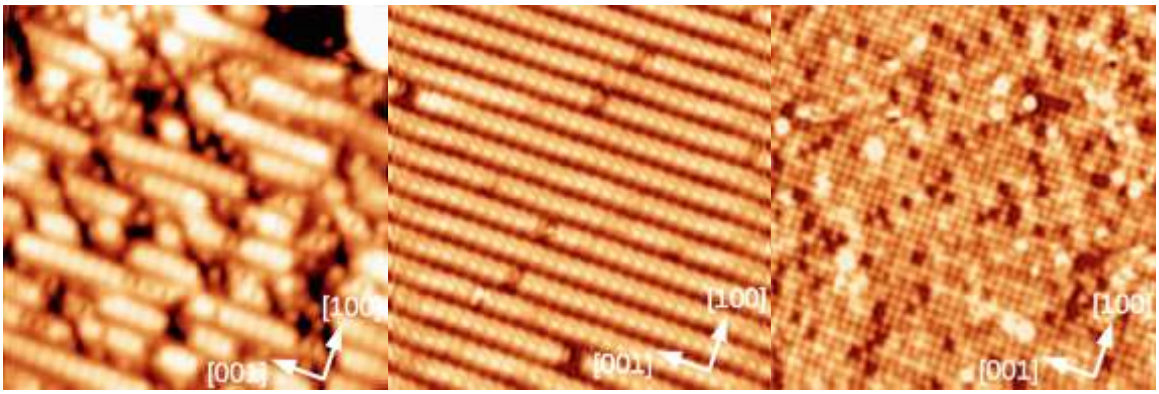
The Al_5Co_2 compound is a promising candidate as new catalyst for the semi-hydrogenation of acetylene. Before investigating its surface reactivity, a detailed study of its surface structure is mandatory. Here, the structural investigations of the (210) and (100) surfaces of Al_5Co_2 using experimental ultra-high vacuum techniques and *ab initio* computational methods will be presented.

The combination of LEED, STM and *ab initio* calculations, including evaluation of surface energies and simulations of STM images gives many arguments towards the identification of the surface structure as bulk truncated terminations where only specific sets of atoms remain. These sets of atoms result from truncations of 3-dimensional chemically bonded atomic clusters, which have been identified in the bulk [1, 2].



(a) (b) (c)

STM images of the Al_5Co_2(100) surface prepared at: 823 K (20x20 nm^2; -2V; 0.1 nA) (a), 973 K (20x20 nm^2; -2V; 0.2 nA) (b), 1043 K (30x30 nm^2; -2V; 0.08 nA) (c).

In this presentation, the interplay between the 2-dimensional surface structures and the 3-dimensional cluster substructure will be discussed, and the results will be compared to similar ones obtained for the Al_5Co_2(001) surface [1]. Surface terminations may also depend on preparation conditions such as the annealing temperature, as seen in Fig. 1 for the (100) surface.

[1] A. Ormeci and Y. Grin, *Isr. J. Chem.* **51**, 1349 (2011).
[2] M. Meier *et al.*, *Phys. Rev. B* (submitted).