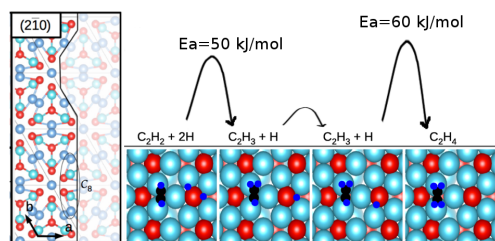


Al₅Co₂ surfaces : from structure to chemical reactivity

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Al₅Co₂(2 $\bar{1}0$) surface structure (side view, left) and schematic reaction path (right).

Recent advances in heterogeneous hydrogenation catalysis have identified few complex intermetallic compounds, like Al₁₃TM₄ with TM=Co,Fe, as promising candidates for the development of efficient cheap catalytic materials¹. The performances of these catalysts have been ascribed to their specific surface structure, made of small, stable, and well-separated atomic ensembles containing generally an unique active transition metal element.

The Al₅Co₂ compound also presents such structural features, that could make it interesting as an effective catalyst. By combining both surface science techniques under ultra-high vacuum and calculations based on the density functional theory, we identified the surface structure of three low index surfaces². The estimation of adsorption energies for a large amount of possible adsorption sites leads to scaling relations between the adsorption energies of C₂H_x, determined for the first time on complex intermetallic surfaces. A possible reaction path for the semi-hydrogenation of acetylene is proposed on the (2 $\bar{1}0$) surface, starting from a 3-fold adsorption site made of 3 aluminum atoms. The corresponding activation energy of the rate controlling step is calculated to be 60 kJ.mol⁻¹. The activation energy of the rate controlling step towards total hydrogenation is evaluated to be 183 kJ.mol⁻¹, thus suggesting a selective catalyst.

1. M. Armbrüster *et al.*, *Nature Materials* **11** 690 (2012); M. Armbrüster *et al.*, European Patent 09157875.7 (2009)
 2. M. Meier *et al.*, *Phys. Rev. B* **93** 075412 (2016); M. Meier *et al.*, *Phys. Rev. B* **91** 085414 (2015)