Designing catalysts in the atomic scale - correlating the structure and catalytic activity

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Correlating structure and function is fundamental for the design of functional materials. Specifically, the atomic rearrangement within a nanoparticle has a direct effect on its properties and overall performance as a building block. While synthetic efforts have succeeded in producing diverse complex materials, the rational design of new materials is still a challenge. Our approach is using atomic resolution HRTEM to unravel the atomic structure of the particle, therefore allowing the understanding of the growth process and the origin of the functionality of the structures. We believe that by doing so, design rules can be offered to optimize the available nanoparticles for their designated role as functional units.

Here, the formation of ternary compounds of transition metal di-chalcogenides (TMDs) by wet chemistry will be described. Specifically, the doping of TMDs with other transition metals and the impact it has on their catalytic properties for hydrogen production will be presented.

The growth mechanism of nanoflowers nanostructures of TMDs was revealed using electron tomography. Using tomography of the nanostructures at different times of the reactions, we showed that the growth mechanism goes through the formations of amorphous pockets, where each crystalizes into a sponge-like structure in the shape of a nanoflower. This growth mechanism allows for facile doping of the materials by adding the dopants either at the beginning or at the end of the reaction, thus forming a homogenous material or a graded one. We have used this approach to dope MoS_2 with Ru, and significantly improving its catalytic activity towards hydrogen production. In addition, we prepared many ternary compounds, and correlated the composition with catalytic activity.

In addition, we have surveyed the structural defects within the nanoflowers in order to correlate them with the catalytic activity. Typical defect motifs will be shown and discussed. This work aims at correlating the atomic-scale structures with the catalytic activity, and for that goal to be achieved, there is a need to understand the dopant sites and the atomic scale arrangement within the MoS_2 lattice. The use of high resolution electron microscopy with other characterization methods allows first the understanding of the structural features of the materials and thereafter it will serve to understand the origin of catalytic activity.