Catalysis with Bulk Reference Catalysts

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The search for new type of catalysts requires broad overview on already studied systems, input from theoretical calculations, chemical intuition and reliable characterization data. The consideration of the catalysts for the application defines also other boundary conditions, which those material should fulfil, e.g. large surface area, well-defined morphology, preferred particle size, specific features of support. Additionally, under operational conditions, many of these parameters vary during the course of reaction, influencing the catalyst performance. The complexity of such systems requires the reliable well-defined (in terms of composition, structure, etc.) reference materials. Such bulk reference catalysts will allow not only to compare the catalytic response, but also to explore the library of experimental data and track the possible changes of the catalyst material under operational conditions.

The catalyst search for the industrially-relevant semi-hydrogenation of acetylene process is selectivity-driven and attracts a lot of attention in catalysis community during the last decades. The novel concept of *laterally condensed catalysts* (LCC), introduced within the CatLab project, provides the opportunity to obtain homogeneous nano-morphology with well-defined functional and reactive interfaces [1]. In this study, reference bulk Pd-Au catalysts were synthesized, extensively characterized and tested for semi-hydrogenation of acetylene. Since, both Pd and Au crystallize with face-centered cubic structure and are chemically similar, continuous solid solution $Pd_{1-x}Au_x$ (x = 0-1) exists in the binary Pd-Au system [2]. The reference Pd-Au catalysts were synthesized with different ratios of Pd to Au in single-phase form. Due to the larger atomic radii of Au, the refined lattice parameters (a) increase linearly from 3.8927(2) Å (for Pd) up to 4.0792(3) Å (for Au), following the Vegard's rule [3]. WDXS analysis of the compositions agrees well with nominal ones. Detailed spectroscopic characterization of the bulk catalysts in pristine and "post-catalysis" state will be presented and accompanied with the catalytic data in comparison with LCC Pd-Au catalysts. Other examples of bulk reference materials' use will be outlined.

[1] Li, Z. et al., submitted to Nature Commun. 2024; [2] Okamoto, H., Massalski, T.B. in Binary Alloy Phase Diagrams, Ed. T.B. Massalski, ASM International, Materials Park, Ohio 1990, 1, 409; [3] Maeland, A., Flanagan, T.B., Canadian J. Phys. 1964, 42, 2364.