Steering the Catalytic Properties of Intermetallic Compounds and Alloys in Reforming Reactions by Controlled in Situ Decomposition and Self-Activation

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Based on the increasing importance of intermetallic compounds and alloys in heterogeneous catalysis, we explore the possibilities of using selected intermetallic compounds and alloy structures and phases as catalyst precursors to prepare highly active and CO₂-selective methanol steam reforming (MSR) as well as dry reforming of methane (DRM) catalyst entities by controlled in situ decomposition and self-activation. The exemplary discussed examples (Cu₅₁Zr₁₄, CuZn, Pd₂Zr, GaPd₂, Cu₂In, ZnPd, and InPd) show both the advantages and pitfalls of this approach and how the concept can be generalized to encompass a wider set of intermetallic compounds and alloy structures. Despite the common feature of all systems being the more or less pronounced decomposition of the intermetallic compound surface and bulk structure and the in situ formation of much more complex catalyst entities, differences arise due to the oxidation propensity and general thermodynamic stability of the chosen intermetallic compound/alloy and their constituents. The metastability and intrinsic reactivity of the evolving oxide polymorph introduced upon decomposition and the surface and bulk reactivity of carbon, governed by the nature of the metal/intermetallic compound-oxide interfacial sites, are of equal importance. Structural and chemical rearrangements, dictating the catalytic performance of the resulting entity, are present in the form of a complete destruction of the intermetallic compound bulk structure (Cu₅₁Zr₁₄) and the formation of a metal/oxide (Cu₅₁Zr₁₄, InPd) or intermetallic compound/oxide (ZnPd, Cu₂In, CuZn) interface or the intertransformation of intermetallic compounds with varying composition (Pd₂Zr) before the formation of Pd/ZrO₂. The prerequisites to obtain a leading theme for pronounced CO₂ selectivity and high activity will be discussed. Special focus will be put on raising awareness of the intrinsic properties of the discussed catalyst systems that need to be controlled to obtain catalytically prospective materials.