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Critcat – towards replacement of critical catalyst materials by improved nanoparticle control and rational design

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CritCat, a project funded by the Horizon 2020 Framework Programme for Research and Innovation of the European Commission, is aimed towards the replacement of critical catalyst materials by improved nanoparticle control and rational design. Catalytic technology for sustainable energy conversion and storage depends strongly on the use of rare platinum group metals (PGMs), and will therefore be greatly affected by their imminent shortage. The CritCat project is intended to provide solutions for the substitution of PGMs by exploring the properties of ultra-small transition metal (TM) alloy, carbide, phosphide, sulphide and oxide nanoparticles, in order to achieve optimal catalytic performance with earth-abundant materials. The focus of the project is on industrially-relevant chemical reactions and emerging energy conversion technologies, in which PGMs currently play an instrumental role, particularly in the context of hydrogen and synthesis gas fuels. Improvements in the sizes, shapes and surface structures of nanoparticle catalysts will be achieved by using novel cluster/nanoparticle synthesis techniques to produce samples of improved quality, combined with experimental characterization, high-level computer simulations of catalytic reactions and algorithms for large-scale materials screening and machine learning based on theoretical and experimental input.
In this contribution, we will introduce the background and objectives of the CritCat project and present preliminary microstructural investigations on novel ultra-small TM alloy clusters and carbide, phosphide, sulphide and oxide nanoparticle catalysts. Nickel phosphides, for example, are efficient electrocatalysts for the hydrogen evolution reaction (HER). We present the results of a microstructural investigation on the structure and composition of mixed Ni5P4, Ni2P, and NiP2 nanosheets grown on Ni foam. A statistical analysis on the electron diffraction patterns reveals that the Ni5P4 nanosheets are mostly oriented along the [001] zone axis. The electrocatalytic reaction mechanism of the nickel phosphide nanosheets subjected to a catalytic test in 0.5 M H2SO4 is further investigated by using energy dispersive X-ray spectroscopy.