Modelling of multi-component alloy nanoparticles for hydrogen production and storage

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In the context of the increasing concern about the energy crisis and the numerous environmental issues, hydrogen should constitute an important part of our clean and secure energy for the future. This, however, depends on being able to produce it in a clean process and store it more conveniently and safely than in high-pressure containers. At the moment, the cleanest way to produce hydrogen is by water electrolysis. This « green » fuel can then be transferred in electrochemical cells to generate electricity while avoiding unwanted gaz emissions. Clean hydrogen production through electrolysis is however limited by the low efficiency of some of the involved chemical catalytic reactions. In this context, research has focused on the use of multi-component alloy systems, or high entropy alloys (HEA [1,2]). In the form of nanoparticles, they constitute a new generation of catalysts with high potential for improving the performance of catalytic chemical reactions.[3] Not only the production but also the secure storage of hydrogen is a big challenge for researchers. Some of the current work focuses on the storage of hydrogen in solids using the properties of the H-Metal bond in the formation of metal hydrides. In this case, multi-component alloy systems should also provide a significant improvement in storage with respect to pure metal hydrides. Thus the presence of sparse crystallographic phases, offering large storage capacity, or the presence of lattice deformations and numerous interfaces internal to the material should largely favor the formation of hydrides.

The proposed doctorate is aimed at characterizing the impact of dimensionality on hydrogen production and storage potentialities in HEA nanoparticles. During this PhD work, the student will be led to compute multi-metallic nanoparticles, going from bimetallic to multicomponents HEA in order to determine their most favorable structural arrangements and study their stability using molecular dynamics (classical and *ab initio*) and Monte Carlo simulations. These methods require the use of N-body interatomic potentials able to represent correctly the chemical bonding between atoms in the studied systems. Such potentials will be developped thanks to the long lasting experience of the group in this field. Then the study of the interaction (adsorption and/or absorption) of the molecules, in particular hydrogen, with such nanoparticles will be performed within the framework of the density functional theory. Reactions of interest for hydrogen formation will also be investigated (like hydrogen and oxygen evolution reactions). All DFT data, in particular energy landscapes for adsorption and absorption, will also constitute a database for further interatomic potentials or force fields fitting and larger scale simulations (kinetic Monte Carlo and classical molecular dynamics). The work will be performed in close collaboration with the experimental microscopy group of DSI (Prof. O. Ersen).

[1] Cantor, B. et al. Microstructural development in equiatomic multicomponent alloys. Mat. Sci. Eng. A-Struct. 375, p. 213–218 (2004).
[2] Yeh, J. W. et al. Nanostructured high-entropy alloys with multiple principal elements: Novel alloy design concepts and outcomes. Adv. Eng. Mater. 6(5), p. 299–303 (2004).
[3] N. K. Katiyar et al., A perspective in catalysis using high entropy alloys, Nano Energy, 88 (2021) 106261.