O.18 Ab Initio and Machine Learning Driven Research of Superhydrides

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The search of new compact systems for high density energy storage remains an open challenge. In this context, transforming energy to hydrogen and storing it in hydrogenated alloys called hydrides is a very promising way. It has been discovered in the past fifteen years that some of them might reach incredibly high hydrogen concentrations under high pressure, leading to stoichiometries that strongly deviate from those governed by the common chemical rules prevailing at ambient pressure. Such compounds are now called *superhydrides* (for example see [1],[2],[3]). Moreover, some superhydrides are expected to be high-temperature conventional superconductors, some of them having, under pressures above 100 GPa, critical temperatures not so far from room temperature (e.g. yttrium superhydrides [2]).

The study of these new materials under extreme pressure conditions can't be realized by experiments alone due to the huge number of potential candidates, and the difficulty to detect the positions of hydrogen atoms by X-ray diffraction techniques. So as to help the experimentalists focusing on the most promizing systems, methods called Crystal Structure Prediction (CSP) algorithms using Ab-Initio calculations coupled to Machine Learning methods appear to be usefull complementary approaches.

In this context, the superhydrides composed of metal type elements are known as systems containing high hydrogen concentrations ([1],[3]). Moreover, they might be easier to synthetize thanks to the availability of these elements in comparison with rare earth ones. This talk will thus present developed and implemented CSP methods employing ABINIT and Machine Learning Potentials to study some of these systems. In particular, the studies realized to predict new superhydrides for systems composed of copper, manganese, yttrium and iron will be presented.

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