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Theoretical tools for the investigation of hydrogen storage materials – from DFT to machine learning

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The prospect of hydrogen utilization in everyday energy demands led to significant efforts of the scientific community to improve materials for hydrogen production, storage, and utilization. Clean energy solutions rely on efficient and safe hydrogen storage, and storing hydrogen in various materials is possible. However, unsolved issues regarding the operational conditions of these materials, the kinetics of hydrogen release, and the volume and weight of the stored hydrogen per unit mass of material limit practical applications.

Besides the experimental approach in synthesizing and modifying the materials, theoretical tools proved to be highly useful in understanding and designing materials with the required properties. One of the most used quantum mechanical methods for the solid state, the density functional theory (DFT), is reviewed. Over a few decades of development and application of DFT showed it is accurate, reliable, and applicable to determining hydride formation/decomposition trends [1][2], energetics [3], and electronic structure and bonding in the hydride phases [4] [5]. The possibility of tuning the properties of the most attractive hydrides by doping, alloying or mechanical mixing will be addressed from the atomic perspective. In particular, some technologically important

hydrides, including Mg-based hydrides, AlH₃-based complex hydrides, and some intermetallic hydrides, will be addressed.

In addition to DFT, the 4th materials revolution, i.e., incorporating data science tools into materials design offered new perspectives in the last decade. One of the key advantages of these efforts is the open data contained in various repositories, which are available to the scientific community. A data-centered approach and chemical intuition synergy are demonstrated in developing a machine learning model to predict hydrogen absorption enthalpy [6]. Artificial neural network models based on the graph neural networks, including MEGNet [7] and our custom-developed model [6] are used to predict thermodynamical properties of the doped hydrides from the hydride crystal structure or the crystal structure of the metal/intermetallic compound.

References

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