Machine learning exploration of the bonding in metal hydrides

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Developing novel materials for efficient hydrogen/energy storage and conversion is one of the critical components in the research area of renewable energy resources. The application of machine learning models has been successfully used for some time to select materials with specific properties desirable for hydrogen storage. This study uses unsupervised and supervised machine learning tools to investigate the relationships between crystal structure, bonding properties, and hydrogen storage performance of the selected materials. A collection of over 500 Mg-containing hydrogen storage materials from the Materials Project [1] with the corresponding calculated DFT-level properties is used. Based on the atomic composition, crystal structure of the starting intermetallic compounds, and properties related to the charge density distribution, we address the nature and character of the bonds between the atoms.

The starting point of our research is gathering DFT-calculated charge densities for Mg-containing hydrides using the pyRho python package [2] to help us access and transform the charge density of selected materials. Charge density is the underlying property of DFT and carries information about any ground state property. Charge topology analysis gives us access to many material properties i.e. how can crystal structure be divided into basins corresponding to atoms or how much charge can we attribute to individual atoms. Also, knowing the values of the first and second derivative of the charge density scalar field can give us insight into bonding character between interacting atoms. Variety of important properties like bandstructure, optical response or electrical conductivity of the material are accessed by using charge density as the beginning step.

Figure 1. displays charge density of the MgH_2 [1] that is dominantly governed by ionic cohesion. Numerous researches addressed the influence of alloying or doping on the applicability of various Mg-hydrides. The nature of charge density in those compounds dictates important properties, such as the stability of hydride, band gap… The principal component analysis will be applied to the dataset containing the structural, bonding, physical, and chemical characteristics of these crystals in order to achieve feature reduction. Finally, a machine learning model will be proposed based on the selected input features to correlate intrinsic material properties with macroscopic or application-related characteristics.

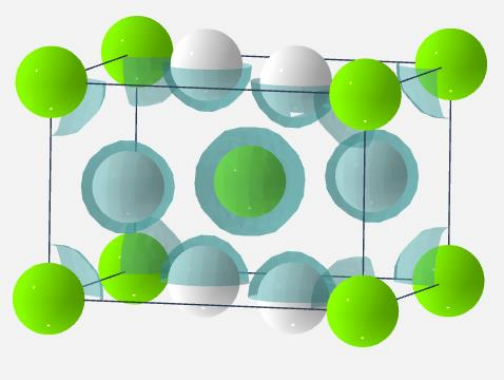

Figure 1. The charge density of MgH_2 [1]. Green spheres – Mg, white spheres – H.

Trends and structure-property relations will be discussed, as well as the possibilities for tailoring the stability of Mg-containing hydrides by alloying based on investigating changes in electronic structure.

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References

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Dr. Bojana Paskaš Mamula received her PhD from the Faculty of Physics, University of Belgrade in 2017. Her research interests include the use of quantum methods for solid state systems that can be used for hydrogen storage and the study of structural and thermodynamic properties of metal hydrides through the use of machine learning models.
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