Solid-state hydrogen storage: Decoding the path through ML guided experiments

Kavita Joshi[1,2], Ashwini Verma[1,2], Nikhil Wilson[1]
[1]CSIR-National Chemical Laboratory, Pune, Maharashtra, 411008 India
[2]Academy of Scientific and Innovative Research, Ghaziabad, Uttar Pradesh, 201002 India,

k.joshi@ncl.res.in

Abstract (Arial 10)

Hydrogen is the fuel of the future, provided the processes associated with its production, storage, and use are made greener. In many applications, hydrogen is produced on the fly through electrolysis, considering the hurdles related to the economical storage of hydrogen. Indeed, hydrogen storage is a bottleneck in realizing the "hydrogen economy". Even today, solid-state hydrogen storage, the most efficient way of storing hydrogen, stays an open question. Hitting a suitable metal hydride is equivalent to searching for a needle in the stack of hay. Thus, it is unsurprising that not a single metal alloy satisfies all the criteria for its commercialization set by US department of energy. It also underlines the need for innovative and efficient ways to screen the chemical space. Figure 1 compares the potential of hydrogen (as chemical energy stored) with existing fuels and highlights the fact that it cannot be realized because of the limitations imposed by its storage as reflected from the specific density.

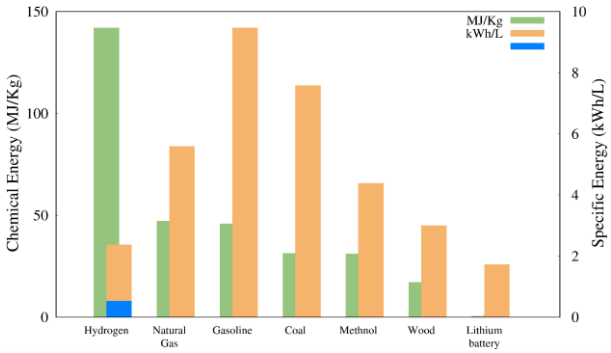

Figure 1: The potential of hydrogen as fuel (reflected in its chemical energy) cannot be exploited because of the existing bottleneck in its storage, which is evident from the specific energy when compared with existing fuels.

In this talk, I will present our journey so far, of searching suitable metal alloys for solid-state hydrogen storage. We have developed various machine-learning models to find the suitability of an alloy to store hydrogen in solid-state. Our models predict H2wt% as a function of absorption temperature and enthalpy of hydride formation.[1] A schematic representation of the workflow of the model is shown in Figure 2. Using these two models, we have scanned ~6.4 million binary, ternary, and quaternary alloy compositions at four different temperatures and filtered ~4000 alloys with H2wt% > 3 at room temperature and enthalpy of hydride formation < 60 kJ/molH_2. Based on our predictions, we have synthesized ternary alloy, which has reversible H2wt% ~ 6.2. [2] The performance of the alloy during hydrogenation and dehydrogenation cycle is shown in Figure 3.

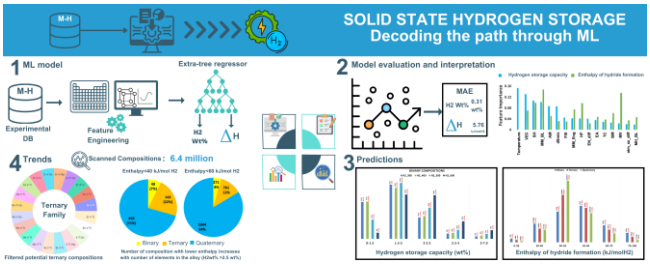

Figure 2. A schematic representation of the ML-based models' workflow.

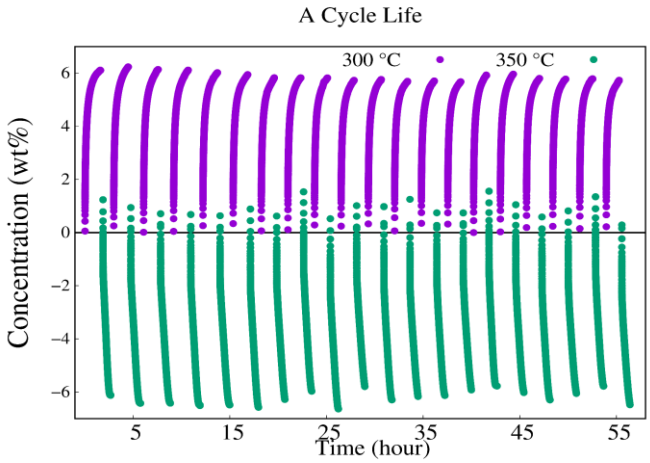

Figure 3: Validating our predictions: Hydrogenation-dehydrogenation cycles of our synthesized alloy.

However, it is not enough to predict the H2wt% and enthalpy of hydrogenation to decide the suitability of alloy. To understand thermodynamic properties of alloys measuring PCT isotherm is a crucial step. However, conducting experiments which includes synthesizing the alloy and then measuring its PCT isotherm is a time-consuming job. Hence, we have developed an ML-based model to predict the PCT isotherm for a given alloy.[3] To train the model, a database of PCT isotherms has also been created from the published literature, which includes 138 distinct alloy compositions and 237 PCT isotherms. Further, a typical result comparing experimental PCT with the ML-predicted is shown in Figure 4.

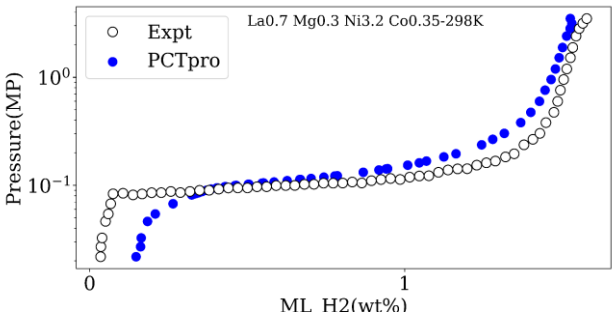

Figure 4. Understanding thermodynamics of an alloy: Predicting PCT isotherm for a given alloy composition. The match between the predicted PCT isotherm and the experimental one is impressive.

References

[1] A. Verma, N. Wilson, and K. Joshi, International Journal of Hydrogen Energy, 50 (2024) 1518-1528
[2] K. Joshi, S. Kumar, A Verma, P. Kumar, Invention disclosure filed [2023-INV-0004]
[3] A. Verma and K. Joshi, “PCTpro: An ML powered PCT isotherm predictor for metal alloys, to be communicated (2024)