THE UNIVERSITY of EDINBURGH
School of Physics and Astronomy

Superconductivity in 3d metal hydrides

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Guilherme Garcia

Supervisor: Prof Andreas Hermann

Introduction

3d metal hydrides (**Mn**, **Fe**, **Co**, **Ni**) have been shown to have superconducting properties at relatively hight T_c. When looking at the different crystal structures of these hydrides some repeat across different metals.

This project aimed to use first principles electronic structure calculations to provide a **systematic study** of this hydrides. We aimed to test known stable structures for one hydride across the range of different metals to look for possible trends. The collected data was used to plot the stability **convex hull** for each of these elements. Once the stable structures have been determined, we attempted to calculate their superconducting T_c .

Methods

In this project we start by using an **example structure from** one of the **literature sources**. This structure is used as an input structure for **VASP** [1]("The Vienna Ab initio Simulation Package") to perform a **structure optimization** across a range of pressures between (0 and 300 GPa). Using the energy of the optimized structures at each pressure point, we plot the convex hull for each of the elements being studied.

Once we have identified the stable compounds for each structure we aimed to perform **phonon calculations** using **Quantum Espresso** [2] in order to determine T_c .

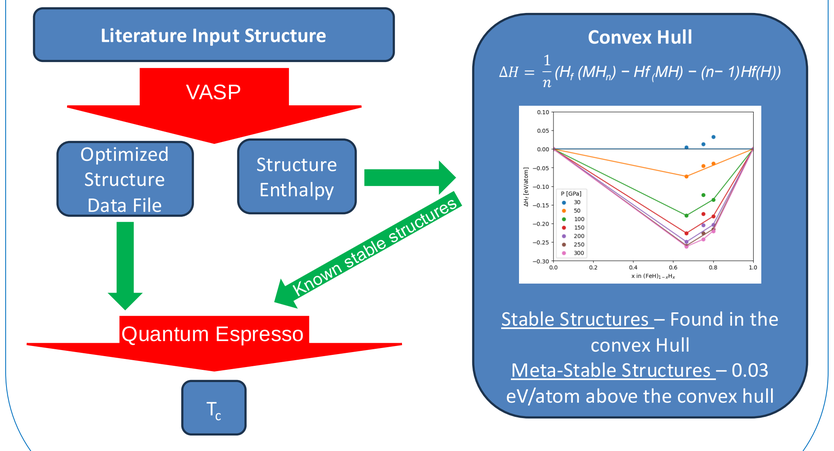

Figure 1: Schematic of the methods used in this study.

Hydrides Convex Hulls

After performing structure optimizations for each structure, we can obtain the convex hull for the hydrides of each metal.

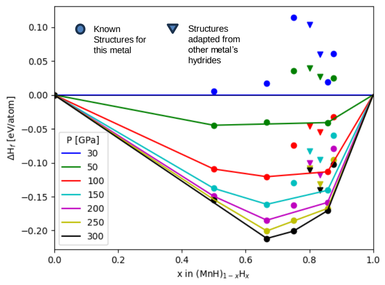

Figure 2: Manganese Convex Hull

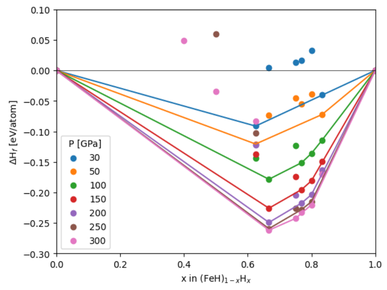

Figure 3: Iron Convex Hull

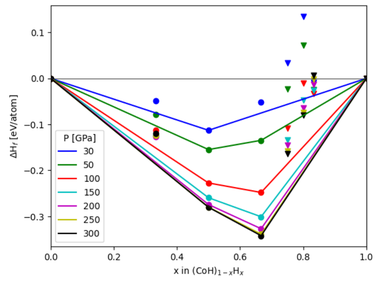

Figure 4: Cobalt Convex Hull

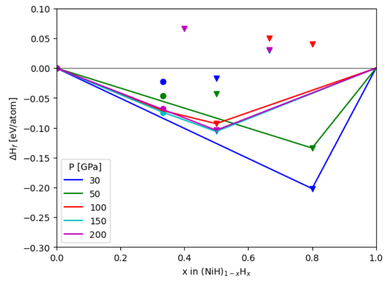

Figure 5: Nickel Convex Hull

Key Results

- Most of the **results for known structures agree with literature**, except for **MnH_8** that should be stable.
- NiH_2 was calculate from an adaption of CoH_2 , which agrees with the literature [3], proofing the **validity of this method**.
- The structure **(Metal)H_5** from Ref.[4] seems to indicate a phase transition into a new stable structure, however when the same structure but from a different literature source is used [5], this is not observed. A more detailed study carried for the MnH_5 seems to indicate that this phase transition leads to an MnH_6 structure, which shouldn't be possible.
- A **new NiH_5 structure** seems to have been found, to confirm it, the (Metal)H_5 structure effect still needs to be excluded.
- Our **T_c calculations were unsuccessful**, returning several negative values for the electron-phonon coupling constant.

Conclusions

This project as tried to provide a comprehensive analysis of the 3d metal hydrides structures and identifying possible trends amongst the hydrides of different hydrides. It identified an interesting phenomena for hydrides of the form **(Metal)H_5** , as well well as a potentially new Nickel Hydride, **NiH_5** .

This opened several avenues that new studies can follow to further explore this topic:

1. A **new T_c calculation** must be attempted to test if new stable structures present superconductivity and at which temperatures. For this, the problems with the phonon calculations be solved. This must include a **structure optimization** step in the Quantum Espresso code to make sure the structures tested are in their stable form and avoid any potential discrepancies that may arise from differences between the VASP and Quantum Espresso code.
2. A more detailed study must be done into the properties of the **(Metal)H_5** structures, what may cause the apparent phase transition and what exactly is the nature of the new structure formed from the transition. This should also check the nature of the NiH_5 form found and confirm its existence by analysing it using inputs from different literature sources.
3. Lastly a further study could focus on **finishing cross-checking the structure forms** that we didn't have time to test on all hydrides in this study as well as conducting a **broader literature review** to find new structures to test.

References

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[3] J. Ying, H. Liu, E. Greenberg, V. B. Prakapenka, V. V. Struzhkin, Physical Review Materials 2, 085409, issn: 2475-9953, (Aug. 31, 2018).
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