

Search for ternary superhydrides metastable at ambient pressure in the Y-Fe-H system: a new prototype structure

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Computational studies have successfully predicted the dramatic uptake of hydrogen by metals under pressure to the formation of superhydrides. These materials demonstrate exceptional properties, such as high-temperature superconductivity, hydrogen storage and superionicity, like in LaH₁₀.^{?,?,?} Up to now, most of the studies have been performed on binary hydrides in the 100 GPa range and none of the discovered superhydrides could be recovered at ambient pressure. Ternary hydrides offer possibilities to stabilize superhydrides at ambient pressure.[?] We have thus undertaken the search of ternary superhydrides in the system Y-Fe-H by coupling calculations and experiments. Remarkably, we synthesized a novel superhydride above 80 GPa that could be recovered metastable at ambient pressure at least for few hours. This is validating a promising avenue for future-experimental investigation in high-temperature superconductivity within hydrides at ambient pressure.

REFERENCES

- [1] M. Somayazulu, et al., Physical Review Letters, Volume 122, page 027001 (2019).
- [2] A.P. Drozdov, et al., Nature, Volume 569, page 528-531 (2019).
- [3] M. Caussé, et al., Phy. Rev. B, Volume 107, page L060301 (2023).
- [4] M. Rahm, et al., J. Am. Chem. Soc., Volume 139, page 8740-8751 (2017).