

# Extracting Measurements from (legacy) publications

HELMHOLTZ AI

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*Helmholtz-Zentrum Dresden Rossendorf, Helmholtz AI / Feb 21, 2024 / LIPS'24*

# Today's Agenda

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1. Motivation
2. Publishing Madness
3. Our Approach
4. Summary

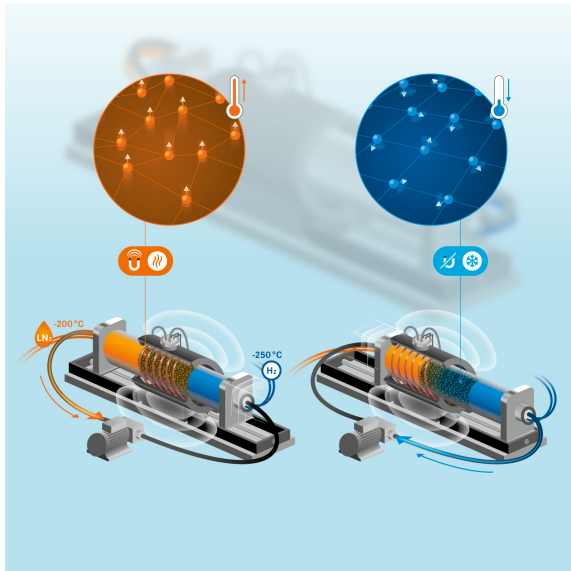
# Motivation

## $H_2$ : energy distribution in a carbon-neutral society



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# Better $H_2$ liquidification: magnetocaloric effect

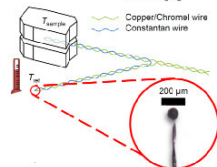
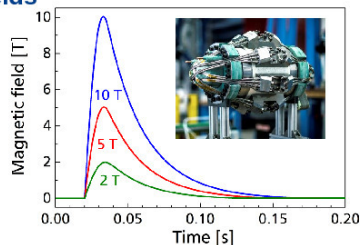
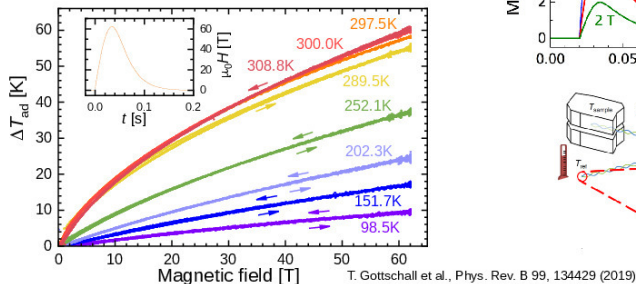


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# Challenge: Find Material that Maximizes Temperature Change at minimal magnetic field expanse

## ■ Single crystal gadolinium in pulsed fields

- 60.5 K maximum  $\Delta T_{ad}$  in 62 T
- No metrological hysteresis
- No eddy-current heating



# Publishing Madness

# Present: People research different material compounds and publish vividly

RESEARCH ARTICLE | AUGUST 04 2015

## Specific heat and entropy change at the first order phase transition of $\text{La}(\text{Fe-Mn-Si})_{13}\text{-H}$ compounds ✓

Vittorio Basso; Michaela Küpferling; Carmen Curcio ; Cecilia Bennati; Alexander Barzca; Matthias Katter; Milan Bratko; Edmund Lovell; Jeremy Turcaud ; Lesley F. Cohen



*J. Appl. Phys.* 118, 053907 (2015)

<https://doi.org/10.1063/1.4928086>

## Role of interplay of austenite and martensite phase fractions on the magnetocaloric and magnetoresistance effects across the martensite transition in $\text{Ni}_{45}\text{Mn}_{44}\text{Sn}_7\text{In}_4$ Heusler alloy near room temperature

Cite as: *J. Appl. Phys.* 128, 215106 (2020); doi: [10.1063/5.0028144](https://doi.org/10.1063/5.0028144)

Submitted: 3 September 2020 · Accepted: 10 November 2020 ·

Published Online: 2 December 2020



## Magnetocaloric properties of $\text{Nd}_x\text{Gd}_{5-x}\text{Si}_4\text{Mn}_{0.5}\text{Cr}_{0.5}$ ( $x = 0.5, 1, 1.5$ )

Eunjeong Kim, Ki Hoon Kang, Chong Seung Yoon 

Division of Materials Science and Engineering, Hanyang University, Seoul, 04763, South Korea



### PAPER • OPEN ACCESS

## On the high-field characterization of magnetocaloric materials using pulsed magnetic fields

To cite this article: C Salazar Mejia *et al* 2023 *J. Phys. Energy* 5 034006



# PDF: a digital form of an analogue paper

IOF Publishing

J. Phys.: Energy 5 (2023) 014006

C. Salazar Maga et al

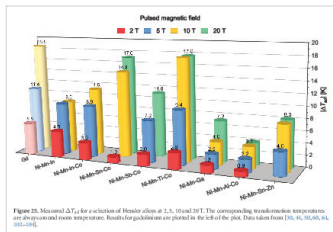


Figure 25. Measured  $\Delta T_M$  for a selection of Heusler alloys at 2.5, 10 and 20 T. The corresponding transition temperatures are displayed on the left of the plot. Data taken from [10, 46, 50, 60, 64, 103–104].

system in the absence of a magnetic field. To return the material to its original state, a mechanical load is applied to shift the hysteresis curve to higher temperatures, and consequently the material transforms back into the low-temperature phase. This process is accompanied by a conventional thermoelectric effect, resulting in a substantial heating effect in the reverse transformation, as indicated (steps 4 and 5). The exact extent of the effect is expected to be the same as in step 6, the final step. The benefit of exploiting the hysteresis in this manner is that the temperature change is not reversed even after the magnetic field is removed, due to the nature of hysteresis.

Heusler alloys seem to be the ideal material class for this kind of application as they possess a tunable transition temperature and large hysteresis. Figure 25 shows the maximum  $\Delta T_M$  values for different Heusler alloys under moderate and high magnetic fields that have been studied at the HLD in the last couple of years [4, 60–62]. We provide comparison with gadolinium as well (conventional refrigeration approach). Amongst the Heusler alloys, the families  $\text{Ni-Mn-Sn}$  and  $\text{Ni-Mn-Sn-Co}$  are outstanding for their large  $\Delta T_M$  in low fields and even reversible effects are obtainable in minor hysteresis loops [100]. The most remarkable one for this is the large shift of the transition temperature in magnetic field  $dT_c/\mu_0\Delta H$ , which can account for  $\sim 10 \text{ K T}^{-1}$  and more in some cases, the means that these materials are only little sensitive for high-field applications as their magnetic transition is already completed in small fields. Furthermore, a large  $dT_c/\mu_0\Delta H$  value results in a reduced entropy change of the complete transition  $\Delta S_{\text{tr}}$  due to the proportionality in the Clausius-Clapeyron equation [101]:

$$\Delta S_{\text{tr}} = -\Delta M \left( \frac{dT_c}{\mu_0\Delta H} \right)^{-1}, \quad (3)$$

where  $\Delta M$  is the magnetization change during the POT. As the entropy change is connected to the temperature via the specific heat, also  $\Delta T_M$  is limited to about 9 K in  $\text{Ni-Mn-Sn}$  independent of the field (see figure 25).

In other Heusler alloys, such as  $\text{Ni-Mn-Sn-Co}$  and  $\text{Ni-Mn-Sn-Ti-Co}$ , the shift of the transition temperature with magnetic field is much smaller implying that higher field change is necessary to complete the transition. For the  $\text{Ni-Mn-Sn-Co}$ —the so-called all-metal Heusler compound—the adiabatic temperature change can achieve 17 K for  $\mu_0\Delta H = 10 \text{ T}$  [64]. During the reconstruction, induced by unloading, the material is warming up by a similar magnitude allowing us to equal the heat to the surrounding. Such a temperature span would be sufficient for the operation of a single-stage multistage air-cooling device at room temperature based on a switching  $\Delta S_{\text{tr}}$ . The key is to properly tune the material properties to the available magnetic-field change with sufficiently large hysteresis at the same time. However,

- often measurements reported in text, graphs, tables
- hard to query automatically (across papers)
- reusing measurements requires human
- my guess: magnetocaloric field too small to warrant community database (by publishers)

# Our Approach

# Retrieval Augmented Generation (RAG) [Lew+20]

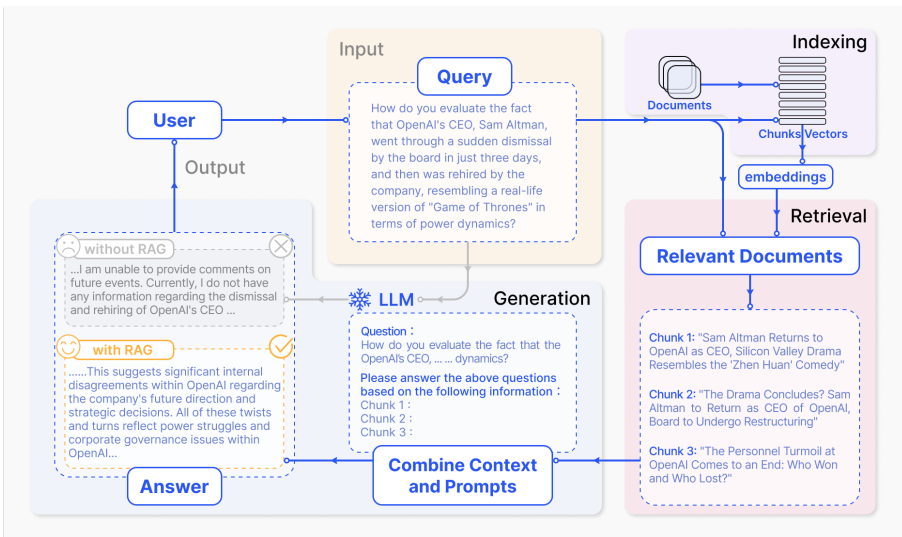


Figure taken from [Gao+24]

# RAG is a super active field!

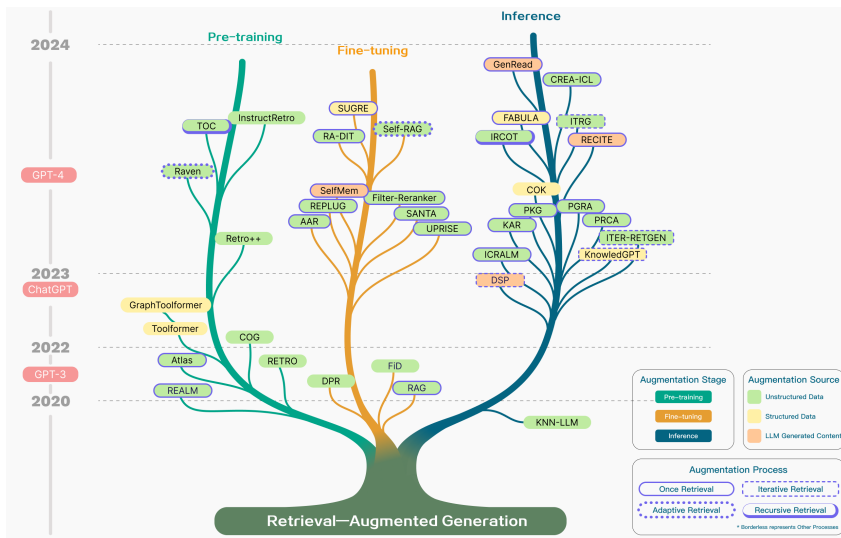


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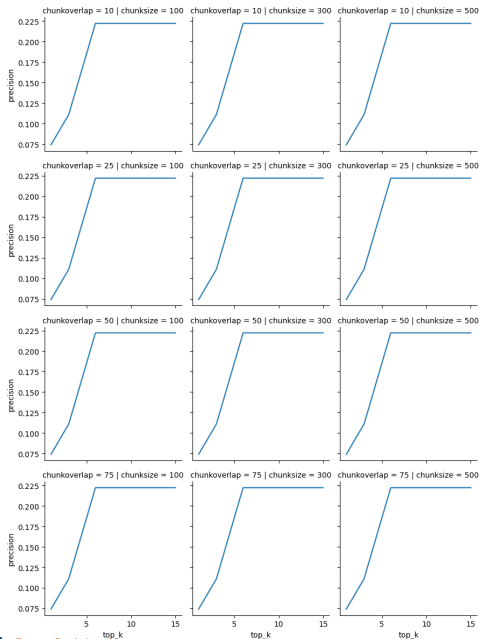
## What we did ...

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- six PDF files from community: created test dataset from these
- use `lagnchain` to facilitate RAG pipeline (chroma DB)
- `sentence_transformer` embedding models (all-MiniLM-L6-v2, all-MiniLM-L12-v2, multi-qa-distillbert-cos-v1)
- **Mistral-7B** LLM hosted by Helmholtz LLM service **blablador**

[helmholtz-blablador.fz-juelich.de](https://helmholtz-blablador.fz-juelich.de)

# Preliminary result: nearest neighbor elbow plot



- as expected: precision increases with increased  $k$
- choose  $k = 6$  as best value
- low precision? test snippets yield varying window sizes between relevant information
- so far: Mistral does not filter nearest neighbor hit list further

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What are the reported values of adiabatic temperature change due to IEM transition?

Based on the provided context, the reported values of the adiabatic temperature change due to the IEM transition are 15.4 K for a magnetic field change from 0 to 5 T at the critical temperature  $T_c=287$  K, and a remarkable value of over 17 K in a 10 T magnetic field without pressure. (Mixtral 8x7b)



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What are the reported values of isothermal temperature change due to IEM transition?

Based on the provided context, the reported value of isothermal magnetic entropy change ( $\Delta S_m$ ) due to the IEM transition is 231 J/kg K in the magnetic field change from 0 to 5 T at a temperature  $T_C = 287$  K for the  $(\text{La}_{0.90}\text{Sr}_{0.10})\text{Mn}_{13}$  compound. For the same magnetic field change and temperature, the indirectly evaluated adiabatic temperature change ( $\Delta T_{ad}$ ) is 15.4 K. However, regarding the  $(\text{La}_{0.90}\text{Sr}_{0.10})\text{Mn}_{13}$  compound, the values of isothermal magnetic entropy change and indirectly evaluated adiabatic temperature change are 230 J/kg K and 12.1 K at  $T_C = 184$  K, respectively. (Mixtral 8x7b)

# Summary

## Wrap-up and call to action

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- RAG appears to be a promising candidate to make LLMs more context aware (and perhaps even safe)
- started to create and validate RAG pipeline given community dataset
- more comprehensive analysis enroute (multiple LLMs, better prompting, better validation)

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### Call to Action

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Thank you for your attention!  
Happy to receive Feedback, Questions or Comments.

# Bibliography I

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- [Gao+24] Y. Gao et al. *Retrieval-Augmented Generation for Large Language Models: A Survey*. 2024. arXiv: 2312.10997 [cs.CL].
- [Lew+20] P. Lewis et al. “Retrieval-augmented generation for knowledge-intensive nlp tasks”. In: *Advances in Neural Information Processing Systems* 33 (2020), pp. 9459–9474.