Search of magnetocaloric materials through machine-learning

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Magnetic ordering in material causes a change in the entropy (ΔS_M), that ends up with a temperature change in solid when a magnetic field is applied or removed (ΔH). This is called magnetocaloric effect, and its one of the alternative path to achieve thermodynamic cycle other than conventional gas[1]. The magnitude of ΔS_M tends to peak at the spontaneous magnetic ordering temperature of a material, such as Curie or Néel temperature, and its maximum value given an applied ΔH strongly depends on the material. Since the discovery of gigantic magnetocaloric effect in materials such as $Gd_5Si_2Ge_2$[2]and $La(FeSi)_{13}$ [3] an explosive increase in the search for materials which could exhibit such effect lead to the accumulation of magnetocaloric properties of a vast number of magnetic materials. However, it remains a challenge the design of materials which can exhibit such remarkable effect. To solve this challenge, we attempted the construction of a machine learning model for the prediction of ΔS_M purely based on the material composition. For this, we gathered the accumulated data of magnetocaloric materials (for instance, ref[1]) and by using the collected data we trained the model for the prediction of ΔS_M given a material composition and an applied ΔH. In Figure 1, we show a model obtained by Random Forest[4].

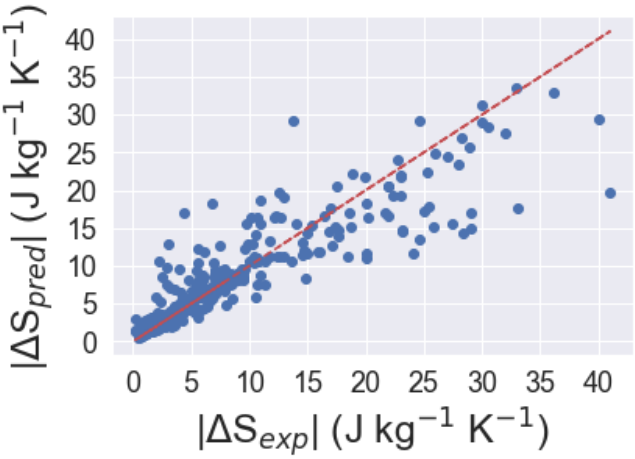

Figure 1. Predictions values versus experimental values for ΔS_M. The blue represents the values predicted by the Random Forest model in our test set. The red line shows the ideal (experimental) values.

In this talk, we would discuss the current status of experimental validation and application of such machine learning model and the challenges that stills need to be solved

References:

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