Discovery of gigantic magnetocaloric effect in HoB_2 guided by 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 the magnetocaloric effect, and it is one of the alternative pathss for the development of refrigeration devices other than the conventional gas-based ones [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 to the design of materials that can exhibit such a remarkable effect.

To solve this challenge, we constructed a machine learning model for the prediction of ΔS_M maximum 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 material composition and an applied ΔH. Then, we explored the text-mined database called MagneticMaterials [4] and used the obtained model in conjunction with the domain expertise to filter possible candidates for experimental verification. By this method, we found that HoB_2 [5] (T_C = 15 K), exhibits that highest volumetric entropy change (0.35 J cm^{-3} K^{-1}), to the best of our knowledge, of all known second-order phase transition materials in the temperature range 4.2 K (T_{LHE}) < T < 77 K (T_{LN2}).

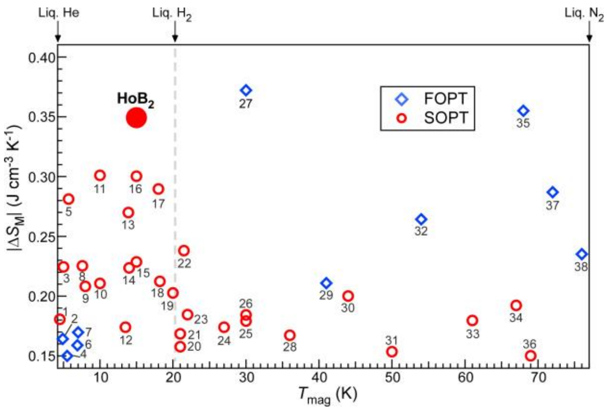

Figure 1 Comparison of the volumetric entropy change of HoB_2 with other materials. Taken from Ref. 5

In this talk, we will discuss the process of model building, the choice of compositional based features, the experimental data of HoB_2, and compare the results to other well known magnetocaloric materials in the same temperature range.

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