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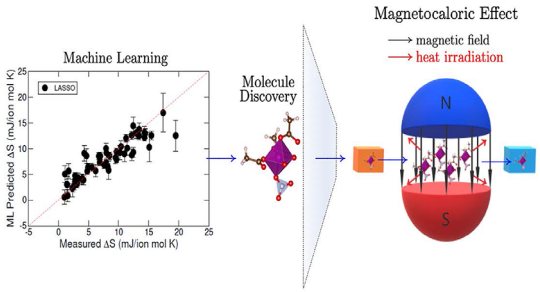
Machine learning models improve design process for new single-molecule magnets by predicting their isothermal magnetic entropy change.



Single-molecule magnets, or SMMs, are polynuclear molecular magnets with potential applications in high-density information storage, magnetic qubits and spintronic devices. They're also a promising material for magnetic refrigeration, which uses the magnetocaloric effect, a temperature change caused by a changing magnetic field to achieve both cryogenic and room temperatures.

Designing new SMMs for magnetocaloric applications is challenging, because there are millions of possibilities, and only a small fraction of these have been experimentally explored. To improve the search for new magnetocaloric SMMs, Holleis et al. turned to machine learning.

Using the 60 known magnetocaloric SMMs, the authors built a dataset and fingerprinted each SMM according to a set of descriptors known to affect isothermal magnetic entropy change, or ΔS_T. ΔS_T is one of the metrics used to measure a material's magnetocaloric performance. A large ΔS_T under small applied magnetic fields is desirable.

The current trial-and-error approach to develop SMMs with preferred properties is time-consuming and expensive. Calculating ΔS_T directly from first-principles method is also inefficient.

The team trained machine learning models to establish a relationship between ΔS_T and SMM descriptors. The models learned to rapidly predict ΔS_T for hypothetical SMMs by identifying key descriptors of SMM that affect ΔS_T, including aspects related to crystal structure and chemistry.

Prasanna Balachandran, one of the authors, said that their work lays the foundation for accelerating the search and discovery of novel SMMs with tailored magnetocaloric properties. The authors expect their models to evolve as training data for their machine learning models grows. They plan to validate their predictions and provide feedback to update and improve their model.

Source: "Machine learning guided design of single-molecule magnets for magnetocaloric applications," by Ludwig Holleis, B. S. Shivaram, and Prasanna V. Balachandran, *Applied Physics Letters* (2019). The article can be accessed at https://doi.org/10.1063/1.5094553.