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Machine learning the magnetocaloric effect in perovskite oxides

This study aims to apply a machine learning methodology to model and predict the magnetocaloric effect in perovskite oxides. A specialized machine learning approach was developed to predict the magnetic entropy change (ΔS_M) of both double and single perovskite oxide materials using data extracted from the literature. A dataset comprising 1 727 entries was constructed using ChatGPT, based on published studies. The input features include composition, synthesis method, crystal structure, space group, particle morphology, lattice parameters (a, b, c), magnetic phase transition type, and transition temperature. Ten machine learning (ML) models were trained using a combination of compositional and experimental features. Both linear and non-linear ML algorithms were employed to predict the negative magnetic entropy change (−ΔS_M) of the materials. Among the evaluated models, the Extra Trees algorithm demonstrated the best performance, achieving an R² score of 0.82. The results provide valuable guidelines for future research on magnetocaloric materials. Furthermore, the methodology is transferable and can be extended to other perovskite-related material domains, such as catalysts and solar cell materials.

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