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Exploring feature generation and engineering techniques for machine learning prediction of ferromagnetic Curie temperatures in perovskites

Majid Shabir Najar[1,†], Muzafar Rasool Bhat[2,†], Assif Assad[3,†], Ghazala Anjum[4,†], Mandeep Singh[1,†] and Farooq Husain Bhat[1,*]

[1] Department of Physics, Islamic University of Science and Technology, Kashmir, Awantipora 192122, India
[2] Department of Computer Science, Islamic University of Science and Technology, Kashmir, Awantipora 192122, India
[3] Department of Computer Science and Engineering, Islamic University of Science and Technology, Kashmir, Awantipora 192122, India
[4] Department of Physics, Govt. SAM Degree College, Budgam 191111, J&K, India

E-mail: farooq.hussain@islamicuniversity.edu.in

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Abstract

Rapid estimation of Curie temperature is essential for discovering advanced functional materials like ABO_3-type ferromagnetic perovskites used in spintronics, sensors, and multiferroics. This study applies machine learning (ML) to predict Curie temperatures directly from chemical formulae, eliminating the need for computationally intensive simulations. A manually curated dataset of 300 perovskites with known Curie temperatures is used. Features are generated by separately considering A-site and B-site cation properties and also by treating the compound as a whole. Three strategies, feature selection, recursive elimination, and principal component analysis are employed for feature engineering. Multiple models are trained and evaluated using cross-validation, with coefficient of determination R^2 as the performance metric. Shapley Additive Explanations highlights mean absolute deviation of A-site ground state volume and B-site space-group number as key factors influencing Curie temperature.

* Author to whom any correspondence should be addressed.
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