INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

Name of the Student	:	SWATI SINGH
Roll Number	:	206103028
Programme of Study	:	Ph.D.

Thesis Title: Machine Learning-Based Design of Critical Raw Material (CRM)-Free Multi-Principal Element Alloys (MPEAs)

Name of Thesis Supervisor(s)	:	Prof. Shrikrishna N. Joshi and Prof. Saurav Goel
Thesis Submitted to the Academic Division	:	Mechanical Engineering
Date of completion of Thesis Viva-Voce Exam	:	08/12/2025
Key words for description of Thesis Work	:	High Entropy Alloys, Machine Learning, Sustainability

SHORT ABSTRACT

This thesis presents a comprehensive, multi-pronged computational strategy for the accelerated and sustainable design of multi-principal element alloys (MPEAs), addressing the challenge of navigating an enormous compositional space (~10^{100} combinations) with limited high-quality experimental data. A machine learning (ML) framework was developed using exclusively experimental data from a consistent synthesis route (melting and casting), avoiding synthetic data augmentation to ensure model robustness and generalizability. Benchmarking revealed that while synthetic augmentation may boost accuracy, it undermines reliability in imbalanced datasets. The resulting framework demonstrated superior generalizability for phase prediction, guiding pre-experimental alloy design. For mechanical property prediction, an open-source toolkit, MAST-ML, was employed to assess the robustness and limitations of standard ML pipelines in this complex materials domain. Insights from this evaluation led to the development of a novel ML–metaheuristic optimization framework that simultaneously optimized yield strength, ultimate tensile strength, and elongation, addressing the longstanding strength–ductility trade-off in MPEAs using ML for the first time.

To promote sustainability, the thesis introduced a dual approach for reducing reliance on critical raw materials (CRMs) or critical and strategic raw materials (C&SRMs). The first approach employed a hybrid ML–optimization framework incorporating CALPHAD-based simulations to identify CRM-lean alloys without compromising mechanical performance. Experimental validation confirmed the viability of these optimized compositions. The second approach proposed strain engineering as a non-compositional, non-ML-based physical design pathway to enhance mechanical properties while minimizing critical material use. Theoretical analysis of literature evidence highlighted mechanisms such as dislocation interactions, grain refinement, and twinning/transformation-induced plasticity (TWIP/TRIP), demonstrating their role in strengthening alloys through process-induced microstructural control. Together, these computational and physical design strategies offer a scalable, sustainable foundation for next-generation alloy development aligned with Net Zero objectives.