Experimentally validated Inverse Design of FeNiCrCoCu MPEAs and Unlocking Key Insights with Explainable AI

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This project developed an integrated computational workflow that combines a **stacked ensemble machine learning** (SEML) model, a convolutional neural network (CNN) model, and evolutionary algorithms to design advanced FeNiCrCoCu multi-principal element alloys (MPEAs) with enhanced mechanical properties. Candidate MPEA compositions predicted through this approach were synthesized and experimentally validated, indicating single-phase face-centered cubic (FCC) structures with mechanical properties (hardness and Young's modulus) qualitatively agreed with the computational predictions. **SH**apley **A**dditive ex**P**lanations (SHAP) analysis provided valuable insights into the computational models, revealing the relationship between elemental concentrations and unstable stacking fault energies in the SEML model, and highlighting correlations between local elemental clustering and mechanical properties in the CNN model. Currently, the workflow from this project is further modified and is being employed to accelerate the design of glycomaterials.

The GlycoMIP supported this research by leading the development of a computational workflow and framework to accelerate materials design. **PARADIM synthesized the new MPEAs and characterized their mechanical properties**.

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Data & Code: Deshmukh-Group/Code_For_XAI_MPEA

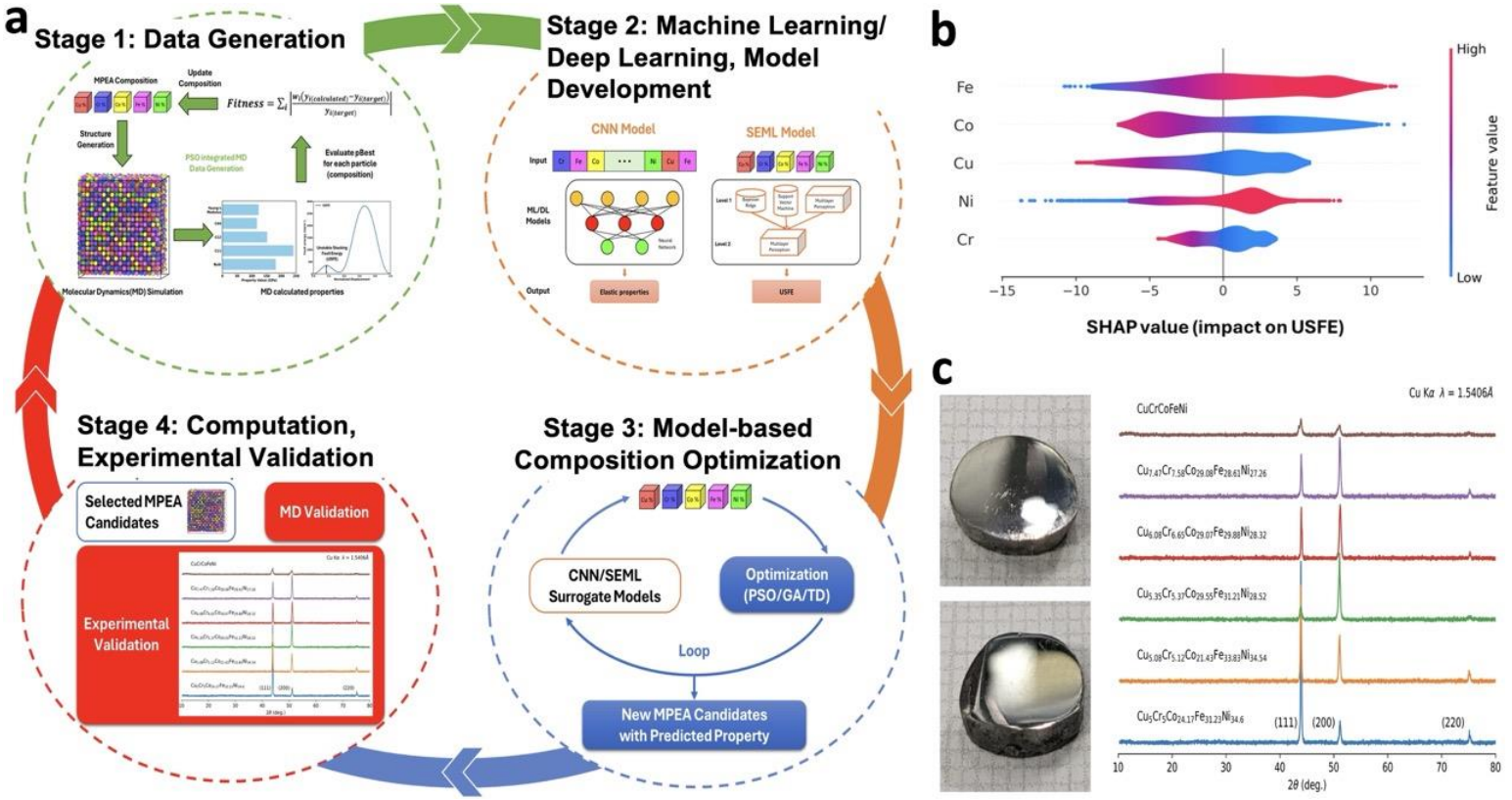

Figure: (**a**) Flowchart of the four-stage hybrid computational workflow. (**b**) SHAP analysis of the SEML model for unstable stacking fault energy (USFE) prediction, revealing the influence of elemental concentrations on the USFE. (**c**) Experimentally synthesized MPEAs, which showed qualitative agreement with computational predictions.