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nimCSO: A Nim package for Compositional Space Optimization

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Summary

The Compositionally Complex Materials (CCMs), and their matal-focused subset of High Entropy Alloys (HEAs), belong to a rapidly emerging class of materials, first proposed by (Cantor et al., 2004) and (Yeh et al., 2004). Contrary to more traditional materials, they contain a large number of chemical elements, typically 4-9 in similar proportions, in hope to thermodynamically stabilize the material by increasing its configurational entropy, by up to $\Delta S_{conf} = \Sigma_i^N x_i \ln x_i$ for ideally random mixing of N elements with fractions x_i.

Statement of Need

Statement of need

Methods and Performance

Methods and Performance

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