High-Entropy Alloy Design Assisted by High-Performance Computing

Michael C. Gao\textsuperscript{1,2}, Jeffrey A. Hawk\textsuperscript{1}, and David E. Alman\textsuperscript{1}
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Ab Initio Molecular Dynamics Simulations

Out of 383 equimolar compositions (4, 5, 6, 7, 8 and 9-components) in each structure, there are 286 FCC compositions, 4 HCP compositions, and 174 BCC compositions that satisfy those constraints.

Entrophy Sources Calculations

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