Ab-Initio Study of the Structural Properties of FeNiCo Medium-Entropy Alloy with Different Local Atomic Environments

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April 2026

Abstract

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A set of special quasirandom structures (SQS) was generated to model chemical disorder and investigate the influence of different local atomic environments on the structural properties of FeNiCo. Self-consistent field (SCF) calculations were performed using Quantum ESPRESSO to obtain energy-volume curves for each configuration at six different lattice parameters. The resulting data were fitted to the third-order Birch-Murnaghan equation of state to determine the equilibrium energy, volume and bulk modulus. The fitted parameters reveal minor variations in the equilibrium lattice parameter with values around 3.46 Å, bulk modulus around 257.71 GPa and the equilibrium energy exhibits subtle differences around −5147.85 eV/atom.

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The 36th Joint NMSU/UTEP Workshop on Mathematics, Computer Science, and Computational Sciences