# Radiation-Resistant High-Entropy Alloys for Space Applications: an Integrated CALPHAD–Molecular Dynamics Study on CoCrFeMnNi

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Radiation tolerance is essential for materials used in satellites and long-duration space missions. High-entropy alloys (HEAs), particularly the Cantor-type CoCrFeMnNi system, offer promising stability and defect resistance under irradiation. In this work, we present an integrated CALPHAD–Molecular Dynamics (MD) framework to evaluate and design radiation-resistant HEAs for space applications.

CALPHAD simulations identified compositional windows that maintain a single-phase FCC structure, with slight Ni enrichment stabilizing phase fields and suppressing brittle intermetallics during rapid solidification typical of additive manufacturing and in-orbit repair. MD simulations of displacement cascades revealed: 30–40 pert lower surviving defect concentrations compared to pure Ni, higher Frenkel pair recombination rates, resistance to cascade-induced amorphization, and retention of tensile ductility even after irradiation.

Together, these results highlight that Ni-enriched CoCrFeMnNi HEAs provide a strong balance of phase stability, defect resistance, and mechanical integrity, making them potential candidates for radiation-tolerant spacecraft structures and shielding. This work demonstrates a simulation-first alloy design pathway for identifying materials with experimental validation for eventual deployment in space environments.