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Ab Initio Studies of Structural, Thermodynamic, Magnetic, and Mechanical Properties of Mn-Ir Alloys

Mn-Ir bimetallic alloys have emerged as promising candidates for spintronic applications due to their attractive properties, such as high thermal stability, large exchange bias fields in Antiferromagnetic/ferromagnetic (AFM/FM) layers. However, the properties of certain phases remain unexplored. In this study, we employed ab initio simulations using the CASTEP code within Materials Studio 2020 with the GGA-PBE functional to investigate the structural, thermodynamic, magnetic, and mechanical properties of disordered L1₀ P4/mmm-MnIr, L1₀ R3m-MnIr, and ordered L1₂ P6₃/mmc-Mn3Ir alloys at 0 K. Our findings reveal that the L1₀ phases exhibit strong magnetism, whereas the ordered L1₂ phase orders zero magnetic moments, a feature that could enhance the intrinsic anomalous Hall effect. Further analysis suggests that the considered MnIr alloys are thermodynamically and mechanically stable. This study provides a valuable insight into the structural, thermodynamic, magnetic, and mechanical properties of disordered L1₀ P4/mmm-MnIr, L1₀ R3m-MnIr, and ordered L1₂ P6₃/mmc-Mn₃Ir alloys.

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