Abstract Submitted
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**First-Principles Study of Phase Stability of *bcc* XZn (X = Cu, Ag, and Au) Alloys**[1] OMAR ALSALMI, MAHDI SANATI , Texas Tech Univ — First-principles density functional theory is used here to study phase stability/instability and anomalies in formation of the *bcc* phases of the aforementioned XZn (X = Cu, Ag, and Au) alloys. The CuZn and AgZn alloys have a disordered *bcc* structure at high temperature; however, this is not the case for the AuZn alloy. The AgZn alloy also has a lower *bcc* order-disorder (critical) temperature compared to CuZn and AuZn alloys. It is shown that these anomalies in *bcc* structure of XZn systems can be explained in terms of the bond strength between the X and Zn atoms. Charge density studies and pair potential modeling of XZn alloys show that the Ag-Zn bond is significantly weaker than the Cu-Zn and Au-Zn bonds. The lattice parameters, bulk modules, elastic constants, Debye temperatures, and heats of formation for the *bcc* phases of the three XZn alloys are calculated and compared with available experimental values.

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