Abstract Submitted
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A First-Principles Study of Structure and Stability of Nickel Carbides JOSH GIBSON, JAMAL UDDIN, University of North Texas, NELLI BODIFORD, University of Texas at Arlington, THOMAS CUNDARI, ANGELA WILSON, University of North Texas — Computational studies of nickel carbides, particularly Ni2C, are scarce. A systematic density functional theory study is reported for Ni2C, along with NiC and Ni3C, to understand the stability and electronic structure of nickel carbides of varying stoichiometry. A comprehensive study was executed that involved 28 trial structures of varying space group symmetry for Ni2C. An analysis of the electronic structure, geometry and thermodynamics of Ni2C is performed, and compared with that for Ni3C and NiC as well as several defect structures of varying composition. It is found that the most stable ground state arrangement of Ni2C exists within a simple orthorhombic lattice and that it has metallic character. The calculated formation energies (kcal/mol) of NiC, Ni2C, and Ni3C are 48.6, 7.9 and 6.4, respectively.

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