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Electronic Structure Properties of Nickel Carbides[1] ANGELA WILSON, JOSHUA GIBSON, THOMAS CUNDARI, University of North Texas — Our analyses of nickel carbides have shown that hexagonal Ni_3C ($\Delta E = 6.4$ kcal/mol) is more stable than NiC ($\Delta E = 48.6$ kcal/mol). To understand the change in stability between these nickel carbides, we have examined the electronic stability and structure of Ni_2C. Using the Vienna Ab-initio Simulation Package (VASP) code, the most stable ground state arrangement of Ni_2C was determined. The total density of states of Ni_2C, the density of states for each nickel and carbon atom within the primitive lattice, and the band structure of Ni_2C were examined. The electronic structure of Ni_2C was compared to those of diamond, NiC (rock salt), and Ni_3C (hexagonal). For Ni_2C, the Fermi energy was obtained and the behavior of the band structure around the Fermi energy was classified. The density of states for nickel and carbon within the relaxed lattice were used to understand the bonding mechanism that exists within Ni_2C.

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