Ab intio study of YNi_4Si under pressure

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In the framework of the density functional theory we study conditions of formation of YNi_4Si compound and its electronic properties under pressure. YNi_4Si has the hexagonal $CaCu_5$ structure with space group P6/mmm. The experimental lattice constants are $a = 4.79$ Å and $c = 4.692$ Å. Within the local density approximation (LDA) used in calculation, the equilibrium volume and the bulk modulus are obtained. The calculated electronic properties reveals changes in the density of states (DOS) under pressure. The theoretical electronic specific heat coefficient γ (14.8 mJ/(f.u. mol K^2)) derived from the density of states at the Fermi energy for the experimental lattice constants and the experimental value of γ (13 mJ/(mol K^2)) are in a reasonable agreement.

In this work we calculate the electronic properties of YNi_4Si under pressure by the self-consistent spin-polarised Tight Binding Linear Muffin Tin Orbital (TB-LMTO) method [1] the atomic sphere approximation (ASA). The systematic errors due to the use of ASA get cancelled-out while determining the ground state energy differences such as formation energy as well as incorporating the so-called 'combined corrections' one can partly salvage the error due to spheridisation of potential and charge density [1, 2]. For the exchange-correlation potential the von Barth-Hedin parametrization [3] has been employed. The Langreth-Mehl-Hu non-local correction [4] was included.

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