Computational Materials Science 49 (2010) 55–59

First-principles study of the thermodynamic properties and electronic structure of compounds from Hf–Ni phase system

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Ab initio calculations of the structural, electronic and thermodynamic properties of Hf_2Ni, HfNi, $HfNi_2$ and $HfNi_5$ are presented. Using all-electron augmented plane waves plus local orbitals (APW+lo) method the relative stability of the selected compounds was determined by calculating their enthalpies of formation and cohesive energies. In addition, their electronic structure and bonding properties were determined. The results are discussed in view of the potential application of these intermetallics as materials for hydrogen storage.