Structures, electronic and thermodynamic properties of NiB2n (n=7-11) and their anions: A theoretical study

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Abstract

Based on the Crystal structure Analysis by Particle Swarm Optimization (CALYPSO) searching method and density functional theory (DFT), theoretical studies about structures, electronic and thermodynamic properties have been investigated systematically at the TPSSh/6-311+G(d) level for NiB2n0/- (n=7-11) clusters. Results found that the lowest energy structures possess a Ni atom-centered double ring tubular boron structures, NiB180/- except. Relative stabilities were analyzed via computing their vertical ionization potentials (VIP), vertical electronic affinity (VEA), adiabatic electronic affinity (AEA), HOMO-LUMO gaps and hardness. The infrared spectra, Raman spectra and photoelectron spectra were computationally simulated to facilitate their experimental characterizations. At last, aromatic properties (Nucleus independent chemical shift) and thermodynamic properties (enthalpy and entropy) with temperature were discussed in detailed for studied systems.

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