# Studies of the physicalproperties of theNowotny–Juza compounds by DFT

***S.Noui1, Z.Charifi2 ,H.Baaziz2***

1Department of physics , Faculty of Science, University of Batna, 05000 Batna, Algeria

2 Department of physics , Faculty of Science, University of M'sila, 28000 M'sila, Algeria

**sameh.noui@gmail.com**

## Abstract

A theoretical study of physical properties of NaZnAs and NaZnSb compounds is presented by performing ab initio calculations based on density-functional theory using the full-potential linear

augmented plane wave (FP-LAPW). The generalized-gradient approximation (GGA) is chosen for the exchange–correlation energy.
The Engel-Vosko (EVGGA) formalism is applied for electronic properties. The calculated structural parameters, such as the lattice constant, bulk modulus and pressure derivative, the electronic band structures and the related total density of states and charge density are presented. The high-pressure β phase of the NaZnAs and NaZnSb is investigated and phase transition pressure from tetragonal to high-pressure phase is determined. We have found that the Nowotny–Juza compounds NaZnAs is direct gap semiconductor and NaZnSb is a metal at ambient pressure. The bonding character and the phase stability of NaZnAs and NaZnSb compounds are discussed.

**Keywords*:*** Electronic materials; Ab initio calculations; Electronic structure; Phase transition; NaZnAs,NaZnSb.