

Half-metallic property of the bulk and (001) surfaces of MNaCs
(M=P, As) half-Heusler alloys: A density functional theory approach

Mohammad Rostami

PII: S0039-6028(18)30038-4
DOI: [10.1016/j.susc.2018.04.006](https://doi.org/10.1016/j.susc.2018.04.006)
Reference: SUSC 21231



To appear in: *Surface Science*

Received date: 17 January 2018
Revised date: 28 March 2018
Accepted date: 10 April 2018

Please cite this article as: Mohammad Rostami , Half-metallic property of the bulk and (001) surfaces of MNaCs (M=P, As) half-Heusler alloys: A density functional theory approach, *Surface Science* (2018), doi: [10.1016/j.susc.2018.04.006](https://doi.org/10.1016/j.susc.2018.04.006)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Highlights

- The electronic and magnetic properties of MNaCs (M=P,As) compounds are considered.
- They are half-metallic ferromagnets with rather high Curie temperatures.
- The half-metallicity is well persevered under stress.
- Atomic magnetic moments at the surfaces are different from the bulk values.
- The bulk half-metallicity is removed at NaCs-terminated (001) surfaces.
- The M-terminated (001) surfaces could preserve the bulk half-metallicity.

Download English Version:

<https://daneshyari.com/en/article/7844744>

Download Persian Version:

<https://daneshyari.com/article/7844744>

[Daneshyari.com](https://daneshyari.com)