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

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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.