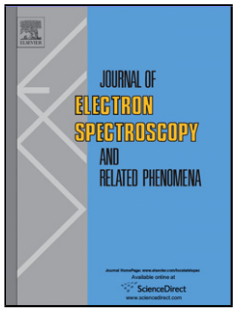

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Electronic and magnetic properties of the (001) surface of the CoNbMnSi Heusler alloy: First-principles calculations

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Highlights

- The half-metallicity verified in the bulk CoNbMnSi is ruined at the (001) surfaces.
- The magnetic moments of Mn and Nb atoms at the (001) surfaces increase, while the atomic magnetic moment of Co and Si atoms decreases.
- The spin-polarization ratio clearly decreases below 75% for (001) surfaces and subsurfaces.

Abstract

In this paper, using first-principles calculations based on density-functional theory, the electronic structures, magnetic properties, and half-metallicity in the bulk and (001) surface of quaternary Heusler alloy CoNbMnSi are studied. For the bulk, the CoNbMnSi compound shows half-metallicity with a band gap of 0.5 eV in the down-spin direction at a equilibrium lattice constant of 5.88 Å. At a similar equilibrium lattice constant, the half-metallicity confirmed in the bulk CoNbMnSi, is ruined at both NbSi- and MnCo-terminated (001) surfaces and subsurfaces. Based on the magnetic property calculations, the magnetic moments of Mn and Nb atoms at the (001) surfaces increase with respect to the corresponding bulk values, while the magnetic moment of Co