Half-metallic properties of KP compound in a bulk and (001) surface of rock-salt structure: A b-initio study

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Abstract
Given the many applications of half-metals in the spintronics devices, we investigated the half-metallic properties of the KP compound in rock-salt (RS) and cesium chloride (CsCl) structural phases by using density functional theory. The results indicated that the KP compound as the half-metal in the RS structure, in contrast to the CsCl structure, due to the small lattice constant and failure of Stoner criterion, did not have any magnetic properties. Half-metallic gap value obtained was remarkable for the RS structure. Although the KP compound in the CsCl structure was more stable than the RS structure energetically, from a dynamical point of view, the RS structure was stable and the CsCl structure was unstable. Calculations corresponding to the (001) surface of the RS structure also demonstrated the conservation of the bulk half-metallic properties in this crystallographic direction. So, the nano-layers of the KP compound in the RS structure might be an appropriate candidate for application in the near future spintronics devices.

Keywords: spintronics, ferromagnetism, half-metal, Stoner criterion, formation energy, cohesive energy

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