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Spin-orbit coupling effect on the electronic structure of Sr_2FeHfO_6 alloy for spintronics application (Article)

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Abstract

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Strong spin–orbit coupling (SOC) in Sr_2FeHfO_6 (SFHO) alloy has been predicted by means of full-potential linear augmented plane wave method in order to study the effect on electronic structure . The tetragonal (I4/mmm) SFHO with SOC has an up-spin energy of ~1.2 eV and a total magnetic moment of ~2.03 μB mainly coming from the Fe (1.63 μB), and the SOC effect was prominent in SFHO due to the magnetic moment of 3d-Fe orbitals. The XAFS spectroscopy technique was used in order to analyze the electronic structure and optical properties of SFHO. The absorption spectra with Fe as a source atom shows a peak appearing around 7118 eV. SFHO with SOC falls within the half metallic state in the up-spin direction resulting significant increase of the total magnetic moment. This half-metallicity strong SOC in SFHO demonstrate much spin polarized electrons around the Fermi level, hence, this material is very potential in future memory devices and spintronic applications. © 2020 Elsevier B.V.

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