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Title:	Optical and electronic properties of double perovskite Ba ₂ ScSbO ₆
Authors:	Ray, Rajyavardhan (/jspui/browse?type=author&value=Ray%2C+Rajyavardhan)
Keywords:	Polycrystalline Perovskite Ba ₂ ScSbO ₆
Issue Date:	2016
Publisher:	American Institute of Physics
Citation:	AIP Conference Proceedings, 1731.
Abstract:	The ordered double perovskite Ba ₂ ScSbO ₆ (BSS) has been synthesized in polycrystalline form by solid state reaction at 1400 C for 72 Hrs. Structural characterization of the compound was done through X-ray diffraction (XRD) followed by Rietveld analysis. The crystal structure is cubic, with space group Fm-3m (No. 225) and lattice parameter, a = 8.20 Å. Optical band-gap has been calculated using UV-Vis Spectroscopy and Kubelka-Munk (KM) function, yielding 4.23 eV. A detailed Ab-initio Density Functional Theory (DFT) study of the electronic properties has been carried out using the Full-Potential Linear Augmented Plane Wave (FP-LAPW) as implemented in WIEN2k. BSS is found to be a large band-gap insulator with potential technological applications.
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