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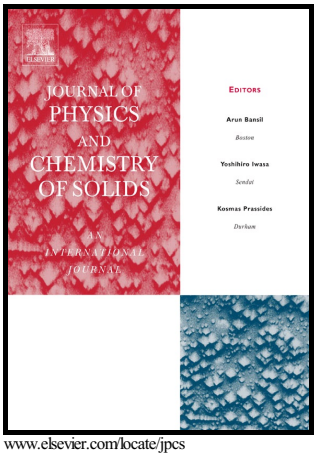

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Electronic properties of Cr-, B-doped and codoped $SrTiO_3$

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Abstract

Spin-polarized density functional theory (DFT) computations have been carried out to investigate Cr-, B-doping as well as codoping in the $SrTiO_3$ crystal. Impact of the oxygen vacancy as an intrinsic point defect has been also taken into consideration. In order to describe more precisely 3*d* electrons of the Ti and Cr atoms, Hubbard-like *U* term in the DFT has been introduced. Outcomes of the calculations reveal occupied states within the forbidden energy region arguing that these in-gap states might be responsible for visible light photocatalysis in the $SrTiO_3$. Structural and magnetic features of the doped and codoped material are discussed as well.

Keywords: $SrTiO_3$; DFT+U; Density of states; Electron localization function.

1. Introduction

Perovskite-type crystals possess numerous properties that make them suitable for a wide range of electronic devices. One of the most prominent perovskite materials is strontium titanate ($SrTiO_3$) crystal, which has attracted many experimental and theoretical studies because of its outstanding applications. Some of its usages include oxygen-gas sensor [1], grain-boundary barrier layer capacitor [2], epitaxial growth substrate for high temperature superconductor (HTSC) thin films [3], and its use as a catalytic material [4].

$SrTiO_3$ is also very promising candidate for being used in the photocatalysis. Production of hydrogen as a fuel by the photocatalysis is environmentally friendly and as a consequence has motivated numerous studies from the scientific community in this field. However, $SrTiO_3$ has a wide band-gap being equal to 3.2 eV [5] that only responds to the ultraviolet light, which is only about 4% of the solar light. Thus, many efforts have been done to overcome this difficulty and to reduce the