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First-principles Study on the Stability and Electronic Properties of Bi-doped $Sr_3Ti_2O_7$

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The electronic and crystal structural properties of Bi-doped $Sr_3Ti_2O_7$ are studied using the first principles density functional theory (DFT) based on pseudopotentials basis and plane-wave method. Our results show that the formation energy of Bi doping in Site-1 and Site-2 of $Sr_3Ti_2O_7$ increases with increasing doping concentration. And at the same doping concentration, the formation energy of Bi doping in Site-2 is lower than that in Site-1. The undoped $Sr_3Ti_2O_7$ is found to be an insulator and its Fermi level stays at the top of the valence band. While the Fermi level of the Bi-doped $Sr_3Ti_2O_7$ moves into the bottom of conduction band, and the system undergoes an insulator-to-metal phase transition. Furthermore, our calculation results demonstrated that the Fermi level of the Bi-doped $Sr_3Ti_2O_7$ goes deeper into the bottom of conduction band with increasing doping concentration.

Keywords: Strontium titanate ceramics; Bi-doping; Phase Stability; Electronic properties; First-principles calculations

1 Introduction

The perovskite-layered oxides, a kind of important functional material, can be applied to many fields, such as superconductivity, thermoelectricity, ferroelectricity and photocatalysis due to their peculiar layered structures and chemical reactivity between the layers. Structure stability, catalytic activity, electronic and thermoelectric