

Electronic Structure of Mg-Doped SrTiO₃ from First Principles

Wen Zeng^{1,2}, Tianmo Liu², Zhongchang Wang¹, Susumu Tsukimoto¹, Yuichi Ikuhara¹

¹ WPI, Advanced Institute for Materials Research, Tohoku Univ., Sendai 980-8577, Japan

² College of Materials Science and Engineering, Chongqing Univ., Chongqing 400044, China

Perovskite oxide SrTiO₃ has nowadays attracted a wide range of attentions because its physical properties are important for many promising applications in the fields of ferroelectricity, grain-boundary barrier layer capacitors, and oxygen gas sensors. Most of these intriguing properties can, however, be altered or improved by doping or solid solution of foreign elements, which is therefore triggering widespread investigations for many technological applications [1,2]. For example, Okhay et al. reported recently that Mg doped SrTiO₃ exhibits a dielectric property without any polar state and attributed structurally this characteristic to the low solubility of Mg on the Sr site in its bulk [3]. However, the mechanism behind this phenomenon has not well been clarified yet from the electronic viewpoint. An understanding of the doping effect of Mg on the electronic and electrical properties of SrTiO₃ especially at the atomic scale is crucial for better control of SrTiO₃ as future functional component [4].

In this work, we applied first-principles calculations to examine the effects of Mg doping on the electronic structure of SrTiO₃. As an initial step towards a general understanding of the origin, the structural, doping formation energy, and electronic property of Mg-doped SrTiO₃ have been investigated and compared with those of pristine SrTiO₃ system (Fig. 1). We find that the Mg atoms locate energetically more stable at Sr site than at the Ti site, which explains the experimental results showing that the Mg prefers to substitute Sr at low temperature. Notwithstanding the easy substitution of Sr by Mg, the electronic structure of SrTiO₃ is found to change insignificantly, as shown in Figs. 2(c) and 3(c). Interestingly, by replacing Ti with Mg, the Fermi level shifts largely to the valence band, which induces acceptor-like state across the valence band of SrTiO₃ (Figs. 2(b) and 3(b)). Similar phenomenon can also be found in the cases of substitution of Ti and Sr atoms by Mg, respectively (Figs. 2(d) and 3(d)), which is in agreement with the experimental study [3]. This dramatic difference of electronic structures between the doping of Mg to Sr and Ti sites is therefore believed to give rise to the distinct electrical performance observed in the experiments. Further examination of how the oxygen defects affect the electronic structures of both undoped and doped SrTiO₃ is still under way, which will be presented in the poster.

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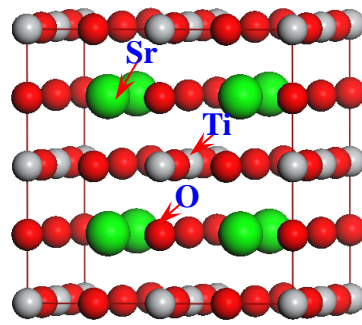


FIG. 1. Schematic illustration of SrTiO₃ models.

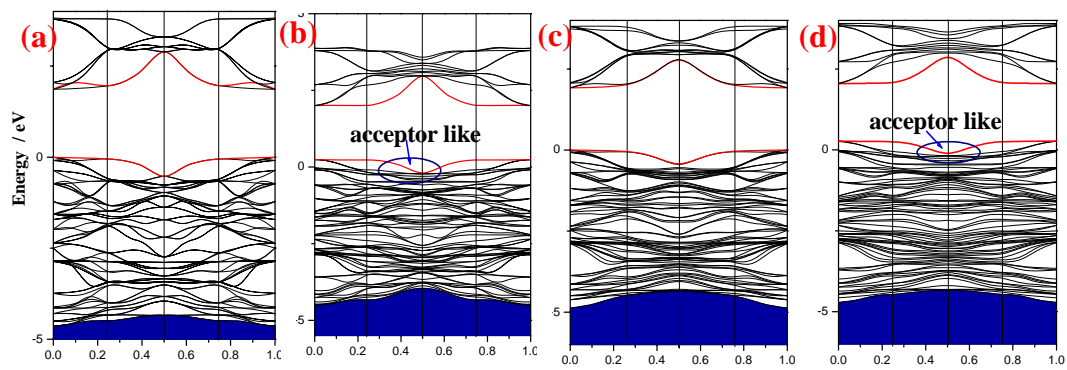


FIG. 2. Band structures of (a) undoped SrTiO₃ and doped SrTiO₃ with Mg substituted at (b) Ti site, (c) Sr site, and (d) both Ti and Sr sites.

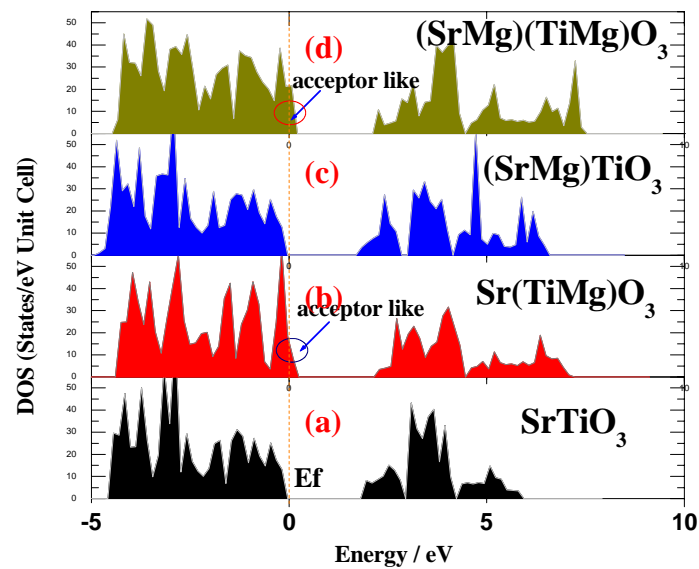


FIG. 3. Density of states for (a) undoped SrTiO₃ and doped SrTiO₃ with Mg substituted at (b) Ti, (c) Sr, and (d) both Ti and Sr sites.