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First-principles calculations for XAS of infinite-layer iron oxides MITSURU KODERA, ISIR, Osaka University, TATSUYA SHISHIDOU, ADSM, Hiroshima University, TAMIO OGUCHI, ISIR, Osaka University — The oxygen defect perovskite $SrFeO_{3-x}$ shows various properties such as the giant magnetoresistance effect and the thermoelectric effect. It had been believed that the oxygen content in $SrFeO_{3-x}$ changes up to $x = 0.5$. Recently, Tsujimoto *et al.* have succeeded in synthesizing the infinite-layer iron oxide $SrFeO_2$. $SrFeO_2$ has a square-planar oxygen coordination, while the iron oxides usually have the tetrahedral and octahedral coordination. $CaFeO_2$ has also infinite layer structure and the same magnetic ordering as $SrFeO_2$. However, it is suggested that the oxygen coordination of $CaFeO_2$ is different from that of $SrFeO_2$. In order to investigate the electronic structure of iron in (Ca, Sr)FeO_2, the x-ray absorption spectroscopy (XAS) spectrum has been measured. In this work, we perform the calculation for XAS spectrum near the Fe-K edge of (Ca, Sr)FeO_2 using the first-principles calculations. We compare the results with the experiment and discuss the electronic structure of iron in (Ca, Sr)FeO_2.

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