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**First-principles calculations for pressure-induced transition of Sr2CuO3** MITSURU KODERA, TAMIO OGUCHI, ISIR, Osaka University — One-dimensional cuprate, $Sr_2CuO_3$ has attracted much attention from the theoretical and material research. Recently, it is found that $Sr_2CuO_3$ exhibits the pressure-induced structural transition with the space group change. In this work, we perform the first-principles calculations in order to investigate the mechanism for the pressure-induced structural transition of $Sr_2CuO_3$. The calculation results are in good accordance with the experimental ones. The structural transition of $Sr_2CuO_3$ are related with the ionic interaction between strontium and oxygen atoms. We also discuss the electronic and magnetic structure of $Sr_2CuO_3$.

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