Electronic Structure of Perovskite Solid Solutions $(\text{SrTiO}_3)_{1-x}(\text{LaTiO}_2\text{N})_x$ \(^1\) NAOTO UMEZAWA, National Institute for Materials Science, ANDERSON JANOTTI, University of California, Santa Barbara — Band gap engineering of oxide perovskite materials is of great interest for electronics and photocatalysis. In this study we demonstrate that the band gap of SrTiO$_3$ is narrowed by mixing it with the oxinitride LaTiO$_2$N. Using hybrid density functional calculations, we study the electronic structure of LaTiO$_2$N and $(\text{SrTiO}_3)_{1-x}(\text{LaTiO}_2\text{N})_x$ solid solutions. We show that the valence-band maximum (VBM) of $(\text{SrTiO}_3)_{1-x}(\text{LaTiO}_2\text{N})_x$ is raised as the LaTiO$_2$N concentration increases, while the conduction-band minimum (CBM) remains almost unchanged. This is explained by the atomic orbitals that composed the VBM and CBM in the two parent compounds: in LaTiO$_2$N the VBM is derived from N 2p states, which are higher in energy than the O 2p that composed the VBM in SrTiO$_3$. The band gap of $(\text{SrTiO}_3)_{1-x}(\text{LaTiO}_2\text{N})_x$ is quantified and discussed in terms of the valence- and conduction-band offsets of SrTiO$_3$/LaTiO$_2$N.

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