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Electronic Structure of Perovskite Solid Solutions $(SrTiO_3)_{1-x}(LaTiO_2N)_x$[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 $LaTiO_2N$. Using hybrid density functional calculations, we study the electronic structure of $LaTiO_2N$ and $(SrTiO_3)_{1-x}(LaTiO_2N)_x$ solid solutions. We show that the valence-band maximum (VBM) of $(SrTiO_3)_{1-x}(LaTiO_2N)_x$ is raised as the $LaTiO_2N$ 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 $LaTiO_2N$ 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 $(SrTiO_3)_{1-x}(LaTiO_2N)_x$ is quantified and discussed in terms of the valence- and conduction-band offsets of $SrTiO_3/LaTiO_2N$.

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