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Magnetic Orders of LaTiO3 and YTiO3 Under Epitaxial Strain: a First-Principles study YAKUI WENG, XIN HUANG, YANKUN TANG, SHUAI DONG, Southeast University — Perovskite RTiO$_3$ family is a typical Mott-insulator with localized 3d electrons. In this work, the epitaxial strain effects on the ground magnetic orders of $LaTiO_3$ and $YTiO_3$ films have been studied using the first-principles density-functional theory. For the $YTiO_3$ films, A-type antiferromagnetic order emerges against the original ferromagnetic order under the in-plane compressive strain by $LaAlO_3$ (001) substrate, although the A-type antiferromagnetic order does not exist in any RTiO$_3$ bulks. Then, for the $LaTiO_3$ films under the compressive strain, e.g. $LaTiO_3$ films grown on $LaAlO_3$, $LaGaO_3$, and $SrTiO_3$ substrates, undergo a phase transition from the original G-type antiferromagnetism to A-type antiferromagnetism. While under the tensile strain, e.g. grown on the $BaTiO_3$ and $LaScO_3$ substrate, $LaTiO_3$ films show a tendency to transit to the C-type antiferromagnetism. Furthermore, our calculations find that the magnetic transitions under epitaxial strain do not change the insulating fact of $LaTiO_3$ and $YTiO_3$.

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