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Intrinsic Insulating Ferromagnetism in Manganese Oxide Thin Films YUSHENG HOU, HONGJUN XIANG, XINGAO GONG, Fudan University, KEY LABORATORY OF COMPUTATIONAL PHYSICAL SCIENCES (MINISTRY OF EDUCATION), FUDAN UNIVERSITY TEAM — Recently, $LaMnO_3$ thin films attract considerable attentions not only because $LaMnO_3$ is the most common magnetic component in all fabricated oxide superlattices/interfaces, but also because experiment observed exotic insulating ferromagnetism in $LaMnO_3$ thin film grown on $SrTiO_3$. However, there is no any model or theory/calculation to explain such striking insulating ferromagnetism. In this work, by means of genetic algorithm optimization, first-principles calculations and the orbital-degenerate double-exchange model studies, we successfully find the insulating ferromagnetic phase of the epitaxially strained $LaMnO_3$ film grown on the cubic $SrTiO_3$ substrate. The unexpected insulating ferromagnetism, which was observed experimentally but not fully understood, originates from the G-type orbital order $d_{3z^2-r^2}/d_{x^2-y}$ and the insulating gap opens as a result of both the orbital ordering and the strong electron-phonon coupling. Our work provides new insight into how a prototypical antiferromagnetic Mott insulator transforms into the ferromagnetic insulator.

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