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Interfacial effects on the electronic structure of LaNiO3 films ZHIGANG GUI, ANDERSON JANOTTI, University of Delaware — $LaNiO_3$ (LNO) is an interesting and unique oxide in the family of perovskite nickelates. For instance, bulk LNO remains metallic and paramagnetic all the way to low temperatures, with no signature of the metal-insulator transition (MIT) and long-range magnetic order as commonly seen in other bulk nickelates. However, MIT has been reported to occur in oxygen-deficient or extremely thin LNO films, the cause of which has been widely debated. Using density functional calculations we study the effects of excess electrons or holes on the electronic and structural properties of LNO bulk and thin epitaxial films. Special attention is paid to interfacial effects, where electrons are transferred to or from LNO thin films through the interfacial termination of the perovskite oxide substrate.

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