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Thickness dependent metal-insulator transition in $GdTiO_3/SrTiO_3$ superlattices[1] ANDERSON JANOTTI, LARS BJAALIE, BURAK HIMMETOGLU, CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — $SrTiO_3$ (STO) is at the core of recent discoveries of two-dimensional electron gas (2DEG) formation at complex oxide interfaces, with the 2DEG residing on the STO side. Experimental results for ultrathin STO layers inserted in $GdTiO_3$ reveal a transition from metallic to insulating behavior, and suggest a strong interplay between electron-electron interaction and lattice distortions. Using first-principles calculations we investigate the evolution of the electronic structure of STO/GTO superlattices as a function of the thickness of the STO layer. We show that the metal-to-insulator transition is a bulk property of STO that emerges at extreme doping levels [1]. For thick STO layers, we find a two-dimensional electron gas with a density of 1/2 electron per unit-cell area per interface within the STO. However, once the STO layer thickness is reduced below three layers, we find that the electrons localize on every second interface Ti atom, giving a charge-ordered Mott-insulating phase. This onset of localization is analyzed in terms of the electron density in the STO layer and octahedral distortions at the interface. The Mott-insulator phase is shown to occur both in $STO/LaAlO_3$ and $STO/GdTiO_3$ heterostructures with ultrathin STO layers.

[1] L. Bjaalie, A. Janotti, B. Himmetoglu, and C. G. Van de Walle, Phys. Rev. B **90**, 195117 (2014).

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