Possible Mott physics in SrTiO$_3$/GdTiO$_3$ superlattices RU CHEN, Department of Physics, University of California, Santa Barbara, CA-93106-9530, SUNGBIN LEE, Department of Physics, University of Toronto, Ontario, Canada, M5S 1A7, LEON BALENTS, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA-93106-9530 — We perform generalized gradient approximation (GGA) + Hubbard U to study the thickness-dependent metal to insulator transition in SrTiO$_3$/GdTiO$_3$ superlattices. A full structural optimization procedure is applied, showing significant electronic and structural reconstruction near the interface between the band insulator SrTiO$_3$ and Mott insulator GdTiO$_3$. In addition, we find high charge density at the interface, close to half electron per interface unit cell (pseudo-cubic notation). For the insulating ultra-thin SrTiO$_3$ layer case, we are able to describe it by a low energy effective Hamiltonian. Using Hartree-Fock approximation, we find the combining effect of the hopping parameters and the correlation in the d orbitals of Ti can lead to possible Mott insulating state. Finally, magnetism is also studied and compared with the GGA+U result.

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