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Metal-insulator transitions in $GdTiO_3/SrTiO_3$ superlattices[1] SE YOUNG PARK, ANDREW MILLIS, Columbia University — The density functional plus U (DFT+U) method is used to obtain electronic structures and metal-insulator phase diagrams of metal-insulator transition of (001) $(GdTiO_3)_m/(SrTiO_3)_n$ superlattices. In metallic phases, the mobile electrons are found in the $SrTiO_3$ layers, with near-interface electrons occupying xy-derived bands, while away from the interface the majority of electrons reside in xz/yz bands. As the thickness n of the $SrTiO_3$ layers decreases a metal-insulator transition occurs. Two insulating phases are found. At $n = 1$ the hybridization of two TiO_2 layers across the SrO layer leads to a dimerized insulating state as previously proposed[2] with relatively small $U_c \sim 2.5$ eV. For $n > 1$ we find that insulating phases occur together with checkerboard charge and orbital ordering and variation of Ti-O bonds at a larger $U_c \sim 3.5$eV. Inconsistencies with experiment suggest that many-body correlations are important.

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[2]Ru Chen, SungBin Lee, and Leon Balents, Phys. Rev. B **87**, 161119(R) (2013).

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