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Metal-insulator transition in nanostructured $SrTiO_3/LaAlO_3$[1]
HOULONG ZHUANG, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, VALENTINO R. COOPER, Materials Science and Technology Division, ORNL, P. GANESH, Center for Nanophase Materials Sciences, ORNL, HAIXUAN XU, Department of Materials Science and Engineering, The University of Tennessee, Knoxville, P. R. C. KENT, Computer Science and Mathematics Division; Center for Nanophase Materials Sciences, ORNL — It is well known that an insulator-to-metal transition occurs at $SrTiO_3/LaAlO_3$ epitaxial heterostructures when the number of $LaAlO_3$ layers reaches a critical value of four. With first-principles calculations, we show that instead of requiring the threshold number of layers to trigger metallicity, the so-called 1+2 overlayer heterostructure also exhibits metallic states. Interestingly, we demonstrate that these metallic states form a two-dimensional electron gas at the overlayer heterostructure. We understand that these fascinating phenomena originate from a modified "polar catastrophe" model, where the overlayer heterostructure accumulates an electrostatic potential more rapidly than regular heterostructures, leading to the reduction of number of LAO layers. Using this model, we further show that the thinner 1+1 overlayer heterostructure exhibits a similar 2DEG. Our work provides a novel approach of inducing 2DEGs in oxide heterostructures, which are beneficial for modern electronics applications.

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