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Atomic-scale control of conductivity in complex oxide thin films

DIVINE KUMAH, ANDREI MALASHEVICH, ANKIT DISA, Yale University, DARIO ARENA, Brookhaven National Laboratory, FRED WALKER, SOHRAB ISMAIL-BEIGI, CHARLES AHN, Yale University — Recent interest in ultra-thin oxide materials such as LaNiO_3 as alternate channel materials for device applications has arisen due to their inherently high carrier densities, as well as the strong coupling of their electronic and magnetic order parameters to structural degrees of freedom. Understanding the structural-property relations in these systems is crucial for designing heterostructure devices for a wide range of applications including Mott field effect transistors. By combining atomic-layer synthesis, picometer-scale 3D imaging using synchrotron x-ray diffraction and first-principles theory, a correlation between the composition and charge of the surface atomic layer of thin LaNiO_3 films and structural distortions which control film conductivity is found. We find that films terminated with positively charged LaO planes preserve bulk-like Ni-O bonding and are metallic. In contrast, films with thicknesses below 5 unit cells terminated with negatively charged NiO_2 -planes are insulating with strongly distorted Ni-O bonds. The differences in the observed structural distortions are understood in terms of a balance between the electrostatic and mechanical boundary conditions governing the two systems.

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