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The Structure of Y_2O_3:ZrO_2 / $SrTiO_3$ Layered Heterostructures MATTHEW DYER, GEORGE DARLING, JOHN CLARIDGE, MATTHEW ROSSEINSKY, The University of Liverpool — Since the discovery of greatly increased conductivity in layered heterostructures of yttria stabilized zirconia (YSZ) and strontium titanate (STO) there has been considerable study and discussion regarding the origin of the high level of conductivity. The detailed atomic structure of layered YSZ-STO heterostructures is likely to be a crucial source of understanding, and as yet remains undetermined, particularly in the region of the buried interfaces between YSZ and STO. We present the results of density functional theory calculations on YSZ-STO heterostructures layered in the [001] direction, with different structures and compositions. We find that structures built using the terminations of the fluorite crystal structure of YSZ do not produce heterostructures which follow conventional solid state chemistry. These heterostructures contain Ti and Zr ions with unlikely O coordination geometries, reduced Ti^{3+} and Zr^{3+} ions and O-O bonding. In contrast, heterostructures built using a reconstructed YSZ termination, based on a rock-salt ordered ZrO layer, give more stable and more conventional atomic structures and are calculated to be electrically insulating. We describe these structures in detail, and the reasons behind the necessary reconstruction of YSZ at the interface.

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