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Mechanisms of Electronic Reconstruction at Oxide Interfaces with 001 and 111 Orientation

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Remarkably rich electronic behavior has been recently discovered at oxide interfaces ranging from two-dimensional conductivity, superconductivity and magnetism to confinement induced metal-to-insulator transitions. Most of the interest so far has been directed at 001 oriented interfaces as e.g. the ones between the two band insulators LaAlO_3 and SrTiO_3 or in superlattices containing the correlated metal LaNiO_3 and the band insulator LaAlO_3 . However, 111 oriented superlattices promise to host even more exotic, possibly topological phases. Despite the difference in stacking with AO and BO_2 planes of the perovskite ABO_3 structure in 001 oriented superlattices versus AO_3 and B layers in the 111 crystallographic direction, analogous effects such as polar discontinuity arise in both cases when the A and B cations are varied across the interface. Based on density functional theory calculations we will compare mechanisms of electronic reconstruction in 001 and 111 oriented superlattices. We will thereby focus on the effect of confinement, band filling, magnetic coupling, structural distortions and substrate strain. Work in collaboration with David Doennig and Warren E. Pickett. Funding by the German Science Foundation, SFB/TR80, is gratefully acknowledged.