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Two Dimensional Electron Gas and Rashba Effect at the Perovskite Polar Surface of $KTaO_3$ S. SATPATHY, K.V. SHANAVAS, Department of Physics & Astronomy, University of Missouri, Columbia — Using density-functional calculations, we study the formation of the 2DEG and the Rashba effect at the polar surface of the perovskite oxide $KTaO_3$, in which the 2DEG has been recently observed [1]. While the formation of the subbands are similar to the polar interface of $LaAlO_3$/ $SrTiO_3$ [2], we find that atomic relaxations play a significant role here in determining its properties. The relaxations substantially weaken the electric field due to the polar structure, reducing electron density at the surface layer. Quite significantly, we find that the lattice relaxations suppress the surface induced asymmetry in the electronic wavefunctions close to the surface, which can explain the lack of significant Rashba splitting in experiments, despite the presence of heavy elements. With a tight-binding model that includes the asymmetry-controlled hopping, we find that the Rashba effect is present only for bands with certain orbital character, allowing for its possible gate control by tuning the occupancies of the various subbands. Density-functional studies with an applied electric field support these results.

[1] P. King *et. al.*, Phys. Rev. Lett., 108, 11602 (2012)
[2] Z. Popović, S. Satpathy, and R. Martin, Phys. Rev. Lett., 101, 256801 (2008)

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