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Charge accumulation in nonpolar perovskite quantum well sandwiched by polar Mott-insulating perovskites CHENG-CHING WANG, University of Texas at Austin, SAHU BHAGAWAN , SWAN, Microelectronics Research Center, HONGKI MIN, WEI-CHENG LEE, MACDONALD ALLAN. H., University of Texas at Austin, CONDENSED MATTER THEORY GROUP AT UT AUSTIN TEAM — We theoretically examine the possibility of having charge accumulation in the $(LaTiO3)_n/Ba2VO4/(LaTiO3)_n$ layered oxide quantum well system with polar barrier material and non-polar quantum well material using a LDA+U approach. The charge accumulation we find reflects electronic reconstruction which tends to occur near polar/nonpolar heterojunctions. We find enormous orbital reconstruction and both antiferromagnetic and ferromagnetic local in different planes. Lattice relaxation in the structure was allowed as a partial test of the robustness of LDA+U predictions for the properties of this system.

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