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Structural and electronic properties of $SrTiO_3/LaNIO_3$ slabs with and without oxygen vacancies PABLO RIVERO, SALVADOR BARRAZA-LOPEZ, JAK TCHAKALIAN, SRIMANTA SMIDDEY, University of Arkansas —
Perovskite oxide heterostructures with transition metal ions exhibit interfacial electronic states completely different to the bulk [1]. Theoretical and experimental researchers are reaching the conclusion that this new behavior emerge as a result of charge redistribution at the interface as a consequence of the polar discontinuity between materials. The creation of Oxygen vacancies [2] is one of the mechanisms known to avoid the electric field divergence, resulting in some cases in high mobility carriers at interfaces. Studying the structural and electronic properties of these compounds with and without Oxygen vacancies could shed more light on the interesting physical phenomena originating at the interface. We use first principle DFT calculations with the LDA exchange-correlation functional to study the formation energy of oxygen vacancies of (5,n) $SrTiO_3/LaNiO_3$ multilayer slab systems, containing n = 1, 2 and 5 layers of LNO. Systems slabs were oriented in the strongly polar (111) direction. We also studied the electronic properties through the electronic density of states (DOS) and the projected full band structure onto the two-oxide interface. We acknowledge computer support from NSF-XSEDE (Project TG-PHY090002. Stampede Supercomputer at TACC). [1] J. Chakhalian, A. J. Millis and J. Rondinelli, Nature Mater. **11**, 92 (2012). [2] G. Herranz, M. Basleti, M. Bibes, C. Carrétéro, E. Tafra, E. Jacquet, K. Bouzehouane, C. Deranlot, A. Hamzi, J.-M. Broto, A. Barthélémy, and A. Fert, Phys. Rev. Lett. **98**, 216803 (2007).

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