

Abstract Submitted
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Two-dimensional electron gas in $\text{NaMnF}_3/\text{SrTiO}_3$ thin films: an *ab-initio* study.¹ WILFREDO IBARRA-HERNANDEZ, ANDRES CAMILO GARCIA-CASTRO, ALDO H. ROMERO, WEST VIRGINIA UNIVERSITY — Control, by surface techniques of the two-dimensional electron gas (2DEG) in oxide/oxide thin-films and heterostructures [1,2], has been one of the most exciting topics recently studied in surface physics. On the other hand, oxide/fluoride heterostructures are expected to be as interesting as the mentioned counterparts. Moreover, our recent findings on A-site geometrically driven ferroelectricity on NaMnF_3 (NMF) under epitaxial strain [3], have motivated experimental efforts to synthesize NMF thin films on SrTiO_3 (STO) substrates. We present *ab-initio* calculations of the electronic and structural properties of these thin-films. We observed the appearance of a 2DEG at the NMF/STO when oxygen or fluorine vacancies are close to the interface. Thin-films without vacancies and intermixing exhibit the appearance of an electric field in STO, in absence of polar-charged layers. This can be explained in terms of the electrostatic potential along the heterostructure induced, and possibly controlled, by the NMF's spontaneous polarization. [1] S. Adhikari, et. al, Adv. Funct. Mater. 26, 5453–5459 (2016) [2] W. Dai, et. al, Nano Lett 16 (4), 2739–2743 (2016) [3] A. C. Garcia-Castro, et. al, Phys. Rev. Lett. 116, 117202 (2016)

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