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A suggestion for making the ferromagnetism at perovskite oxide interfaces robust NIRMAL GANGULI, PAUL KELLY, Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands — LaAlO₃|SrTiO₃ heterostructures have received much attention following observations of ferromagnetism, superconductivity and of an insulator to metal transition at the interface between otherwise conventional band insulators. One of the challenges posed by recent observations is to understand how high mobility charge carriers and local magnetic moments can coexist at n-type interfaces where the lack of a detailed knowledge of the interface structure from experiment is a major impediment to understanding these physical properties. A more extensive first principles study of the ferromagnetically ordered state found for modest values of Hubbard U in the presence of GdFeO₃type octahedral tilts at the interface [1] suggests that it should be possible to make the interface ferromagnetism more robust by enhancing the octahedral tilts. We screened a number of oxide interfaces with first principles calculations and identified the LaAlO₃|CaTiO₃ (001) interface as the most promising candidate in the large charge transfer limit, owing to the large intrinsic tilt of TiO₆ octahedra in CaTiO₃.

[1] Z. Zhong and P. J. Kelly, Europhys. Lett. 84, 27001 (2008)

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