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Ab-initio investigation of ferroelectricity in asymmetrically layered magnetic perovskites ALISON HATT, NICOLA SPALDIN, University of California, Santa Barbara — In an effort to combine magnetism and ferroelectricity in a single material we are motivated to explore creative routes to ferroelectricity that allow the coexistence of magnetism. In this talk we present results from an ab-initio study of a system of asymmetrically layered magnetic perovskite oxides in which the asymmetric layering should induce a ferroelectric polarization. We investigate this prediction in a model system of La(Al,Fe,Cr)O_3, and find that a large switchable ferroelectric polarization can indeed be obtained, although it does not originate from the asymmetric layering. We examine the forces driving polarization in this system, and propose two- and three-dimensional heteroepitaxy as a general route to stabilizing novel ferroelectrics and multiferroics.

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