

Magnetic Properties and Improper Ferroelectricity in $\text{LaFeO}_3/\text{LaCrO}_3$ Superlattices

Q. Zhang^{a, b} and S. Yunoki^{a, b, c}

^aComputational Condensed Matter Physics Laboratory, RIKEN, Wako, Saitama 351-0198, Japan

^bCREST, Japan Science and Technology Agency (JST), Kawaguchi, Saitama 332-0012, Japan

^cComputational Materials Science Research Team, RIKEN AICS, Kobe, Hyogo 650-0047, Japan

First-principles calculations have been performed to investigate the electronic and magnetic properties of $\text{LaFeO}_3/\text{LaCrO}_3$ superlattices. It is found that the magnetic structures of $[\text{LaFeO}_3]_n[\text{LaCrO}_3]_m$ superlattices are much sensitive to the stacking direction and to the stacking periodicity of (n,m). In the case of superlattices with (1, 1), the magnetic ground states of the systems growing along [001] and [110] directions are C-type and A-type antiferromagnetic insulators, respectively, whereas a ferromagnetic insulator is achieved when Fe and Cr layers are atomically stacked along [111] direction. In the case of superlattices with (2, 2) and (3, 3) growing along [001] direction, Fe layers are ferromagnetically coupled with the nearest neighboring Cr layers, while Fe (Cr) layers are antiferromagnetically coupled with the adjacent Fe (Cr) layers. These results are consistent with Konamori-Goodenough (KG) rule, and are in good agreement with experimental observations. Furthermore, we predict that the superlattice with (2, 2) growing along [110] direction is E-type antiferromagnetic insulator with finite ferroelectric polarization, namely, the system is multiferroic.