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Theoretical Investigation of the Origin of Interfacial Ferromagnetism of $(LaNiO_3)n/(CaMnO_3)m$ Superlattices

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Abstract : Metal to insulator transition and interfacial magnetism of the $LaNiO_3$ based superlattice are main interest due to thickness dependent electronic response and tunable magnetic behavior. We investigate the structural, electronic, and magnetic properties of recently experimentally synthesized $(LaNiO_3)n/(CaMnO_3)m$ superlattices with varying $LaNiO_3$ thickness using density functional theory. The effect of the on-site Coulomb interaction is discussed. In switching from zero to finite U value for Ni atoms, $LaNiO_3$ shows transitions from half-metallic to metallic character, while spinning ordering changes from paramagnetic to ferromagnetic (FM). For $CaMnO_3$, $U < 3$ eV on Mn atoms results in G-type anti-FM spin ordering whereas increasing U value yields FM ordering. In superlattices, metal to insulator transition was achieved with a reduction of $LaNiO_3$ thickness. The system with one layer of $LaNiO_3$ yields insulating character. Increasing $LaNiO_3$ to two layers and above results in the onset of the metallic character with a major contribution from Ni and Mn 3d eg states. Our results for interfacial ferromagnetism, induced Ni magnetic moments and novel antiferromagnetically coupled Ni atoms are consistent with the recent experimental findings. The possible origin of the emergent magnetism is proposed in terms of the exchange interaction and Anderson localization.

Keywords : density functional theory, interfacial magnetism, metal-insulator transition, Ni magnetism.
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