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Effective of charge doping in the $LaNiO_3/SrTiO_3$ superlattices[1]
HEUNG-SIK KIM, MYUNG JOON HAN, Department of Physics, Korean Advanced Institute of Science and Technology, Daejeon, Korea — In this study we investigate the charge doping effect on the crystal and electronic structure of $LaNiO_3/SrTiO_3$ superlattice with density-functional theory calculations. It is found that the doped charge favors Ni $d_{3z^2-r^2}$ orbital, and that the NiO_6 octahedron is elongated or compressed along the z-direction in order to reduce the energy. Under the fixed in-plane lattice constant, the octahedral distortion upon charge doping can be understood as a doping-induced effective epitaxial strain. The rotation of the NiO_6 octahedra is affected by the charge doping and the resulting doping-induced effective strain. Inclusion of the electron correlations enhances the orbital-lattice coupling and the structural changes. Possible cuprate-like Fermi surfaces induced by hole doping will also be discussed. Our work provides insights on the effect of charge doping on the nickelate superlattices, and suggests a doping-controlled structural evolution in these systems.

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