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Modulation doping in $LaNiO_3/SrIrO_3$ superlattices from first principles[1] MICHELE KOTIUGA, HEUNG-SIK KIM, DAVID VANDERBILT, KARIN M. RABE, Department of Physics and Astronomy, Rutgers University —
Doping is commonly used to tune and optimize material properties such as conductivity and optical properties. Doping at extremely high concentrations, at the level of an electron per formula unit, can stabilize novel phases. Here we study lanthanum nickelate ($LaNiO_3$)/strontium iridate ($SrIrO_3$) superlattices using the first-principles density functional theory (DFT) +U method, focusing on the 1/1 superlattice. For this superlattice we find that there is a complete modulation doping in which one electron per formula unit is transferred from the $SrIrO_3$ layers to the $LaNiO_3$ layers, converting all nickels from Ni^{3+} to Ni^{2+} in the electron-doped $LaNiO_3$ layers and and all iridiums from Ir^{4+} to Ir^{5+} in the hole-doped $SrIrO_3$ layers. We will present results on the low energy structures and orbital occupations as well as the electronic and magnetic structures.

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