Abstract Submitted for the MAR17 Meeting of The American Physical Society

Spin-Orbital entangled 2DEG \mathbf{in} the δ -doped interface $La_{\delta}Sr_{2}IrO_{4}$: Density-Functional Studies and Transport Results from Boltzmann Equations CHURNA BHANDARI, ZORAN POPOVIC, SASHI SATPATHY, University of Missouri - Columbia — The strong spin-orbit coupled iridates are of considerable interest because of the Mottminsulating state, which is produced by the combined effect of a strong spin-orbit coupling (SOC) and Coulomb repulsion. In this work, using density-functional methods, we predict the existence of a spin-orbital entangled two dimensional electron gas (2DEG) in the delta-doped structure, where a single SrO layer is replaced by an LaO layer. In the bulk Sr_2IrO_4 , a strong SOC splits the t_{2g} states into $J_{eff} = 1/2$ and 3/2 states. The Coulomb repulsion further splits the half-filled $J_{eff} = 1/2$ bands into a lower and an upper Hubbard band (UHB) producing a Mott insulator. In the δ -doped structure, La dopes electrons into the UHB, and our results show that the doped electrons are strongly localized in one or two Ir layers at the interface, reminiscent of the 2DEG in the well-studied LaAlO₃/SrTiO₃ interface. The UHB, consisting of spin-orbit entangled states, is partially filled, resulting in a spin-orbital entangled 2DEG. Transport properties of the 2DEG shows many interesting features, which we study by solving the semi-classical Boltzmann transport equation in the presence of the magnetic and electric fields.

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Date submitted: 10 Nov 2016

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