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First-principles study of $\text{Sr}_2\text{Ir}_{1-x}\text{Rh}_x\text{O}_4$: charge transfer, spin-orbit coupling change, and the metal-insulator transition¹ JAE-HOON SIM, Department of Physics, KAIST, Daejeon 305-701, Korea, HEUNG-SIK KIM, Department of Physics, University of Toronto, Toronto, Ontario M5S 1A7, Canada, MYUNG JOON HAN, Department of Physics, KAIST, Daejeon 305-701, Korea — Using first-principles density functional theory (DFT) calculations, we investigated the electronic structure of Rh-doped iridate, $\text{Sr}_2\text{Ir}_{1-x}\text{Rh}_x\text{O}_4$ for which the doping (x) dependent metal-insulator transition (MIT) has been reported experimentally and the controversial discussion developed regarding the origin of this transition. Our DFT+U calculation shows that the value of $\langle L.S \rangle$ remains largely intact over the entire doping range considered here ($x = 0.0, 0.125, 0.25, 0.50, 0.75, \text{ and } 1.0$) in good agreement with the branching ratio measured by x-ray absorption spectroscopy. Also contrary to a previous picture to explain MIT based on the charge transfer between the transition-metal sites, our calculation clearly shows that those sites remain basically isoelectronic while the impurity bands of predominantly rhodium character are introduced near the Fermi level. As the doping increases, this impurity band overlaps with lower Hubbard band of iridium, leading to metal-insulator transition. The results will be discussed with comparison to the case of Ru doping.

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