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Spin-Orbit Coupling Assisted Mott Insulator Sr_2IrO_4 S. J. MOON, J. S. LEE, M. W. KIM, T. W. NOH, ReCOE & FPRD, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea, H. JIN, B. J. KIM, J. YU, S.-J. OH, CSCMR & FPRD, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea, J.-H. PARK, Pohang Accelerator Laboratory, Postech, Pohang 790-784, Korea, C. KIM, Institute of Physics and Applied Physics, Yonsei University, Seoul, Korea, G. CAO, Department of Physics and Astronomy, University of Kentucky, Lexington, Kentucky 40506, USA — We have systematically investigated the effect of spin-orbit coupling to the optical conductivity spectra $\sigma(\omega)$ of Sr_2IrO_4. Both Sr_2RhO_4 and Sr_2IrO_4 have five d electrons and similar crystal structures. However, Sr_2RhO_4 and Sr_2IrO_4 are metallic and insulating, respectively. The insulating ground state of Sr_2IrO_4 is rather surprising, since it has $5d$ electrons, which are commonly thought to have extended orbitals. We observed a sharp absorption at about 0.5 eV in $\sigma(\omega)$. This spectral feature cannot be explained in terms of orbital degeneracy and/or density wave. Note that Ir has $5d$ electrons, so that its spin-orbit coupling should be larger than that of $4d$ Rh ions. With the aid of the first principles calculation based on the LDA+U scheme, we took into account of the effect of spin-orbit coupling. Our results clearly demonstrate that spin-orbit coupling plays a crucial role to the Mott insulating ground state of Sr_2IrO_4.

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