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Spin-orbit coupling triggered Mott insulator Sr_2IrO_4. BUM JOON KIM, HOSUB JIN, SOON JAE MOON, JAE-YOUNG KIM, CHOON SHIK LEEM, JAEJUN YU, TAE-WON NOH, CHANGYOUNG KIM, SE-JUNG OH, JAE-HOON PARK, GANG CAO — Electronic structures of 5d transition-metal oxide (TMO) $Sr_2IrO_4$are investigated by angle-resolved photoemission spectroscopy and density-functional electronic structure calculations. The insulating nature of this compound and its measured valence band symmetry are correctly accounted for by the calculation only when both spin-orbit coupling and electronic correlation effects are included. It is shown that the spin-orbit coupling plays a crucial role in stabilizing the Mott-insulating ground state, which is unexpected in a compound with extended 5d valence band. The spin-orbit coupling leads to symmetry-split-off bands near the Fermi level which are narrow enough to be gapped by the Coulomb repulsion of moderate strength. This results in a conduction band as narrow as $\sim$0.5 eV, defying its general character expected for $5d$ TMO. Our finding marks an establishment of a new type of Mott insulator and suggests possibility of novel Mott-derived phenomena in $5d$ based materials.

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