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Manifestation of on-site Coulomb and spin-orbit interactions in the ground state electronic structure of Sr_2IrO_4 HOSUB JIN, JAEJUN YU, Seoul National University — In contrast to the superconducting and metallic ground states in Sr_2RuO_4 and Sr_2RhO_4, the ground state of Sr_2IrO_4 has been reported to be a magnetic insulator. Such an insulating character of Sr_2IrO_4 is rather surprising and unexpected when the extended nature of Ir $5d$ state is considered. To investigate the electronic structure of Sr_2IrO_4, we performed LDA+U calculations taking account of spin-orbit interactions, where both on-site Coulomb interactions and spin-orbit couplings in the description of Ir 5 d states are expected to play a significant role. From the results, it is shown that neither the on-site U nor the spin- orbit term only can explain the insulating feature of Sr_2IrO_4. An interesting interplay between the two competing interactions is found to determine the spin and orbital configuration, leading to a novel insulating ground state. To understand the nature of the ground state, we suggest a minimal model for the t_{2g} manifold based on the tight binding Hamiltonian.

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