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Large Band Gap of alpha-$RuCl_3$ Probed by Photoemission and Inverse Photoemission Spectroscopy SOOBIN SINN, CHOONG HYUN KIM, LUKE SANDILANDS, IBS-CCES, Seoul National University, KYUNGDONG LEE, CHOONGJAE WON, IBS-CCES, Inha University, JI SEOP OH, IBS-CCES, Seoul National University, MOONSUP HAN, YOUNG JUN CHANG, University of Seoul, NAMJUNG HUR, Inha University, HITOSHI SATO, Hiroshima Synchrotron Radiation Center, BYEONG-GYU PARK, Pohang Accelerator Laboratory, CHANGYOUNG KIM, HYEONG-DO KIM, TAE WON NOH, IBS-CCES, Seoul National University — The Kitaev honeycomb lattice model has attracted great attention because of its possibility to stabilize a quantum spin liquid ground state. Recently, it was proposed that alpha-$RuCl_3$ is its material realization and the first $4d$ relativistic Mott insulator from an optical spectrum and LDA+U+SO calculations. Here, we present photoemission and inverse photoemission spectra of alpha-$RuCl_3$. The observed band gap is about 1.8 eV, which suggests that the previously assigned optical gap of 0.3 eV is misinterpreted, and that the strong peak at about 1.2 eV in the optical spectrum may be associated with an actual optical gap. Assuming a strong excitonic effect of 0.6 eV in the optical spectrum, all the structures except for the peak at 0.3 eV are consistent with our electronic spectra. When compared with LDA+U+SO calculations, the value of U should be considerably larger than the previous one, which implies that the spin-orbit coupling is not a necessary ingredient for the insulating mechanism of alpha-$RuCl_3$. We also present angle-resolved photoemission spectra to be compared with LDA+U+SO and LDA+DMFT calculations.

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