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The Mott Insulating Nature of Na_2IrO_3 : DFT+DMFT Study

MINJAE KIM, CPHT, Ecole Polytechnique College de France, BEOM HYUN KIM, RIKEN, Saitama, B. I. MIN, Pohang University of Science and Technology — We have investigated the insulating nature of Na_2IrO_3 , employing both the density-functional theory (DFT) and the combination of the DFT and the dynamical mean-field theory (DFT+DMFT). We have obtained the paramagnetic (PM) insulating state even above the Neel temperature (T_N), which reveals that Na_2IrO_3 is a Mott-type insulator. The photoemission spectrum is well described by the density of states from the DFT+DMFT in this PM insulating state. However, the analysis of optical conductivity suggests that the non-local correlation effect is also important in Na_2IrO_3 . We have also found sizable redistribution of both charge and spin densities upon cooling below T_N which suggests that Na_2IrO_3 is not a standard Mott insulator having rigid charge density. Therefore, despite the Mott-type insulating state of Na_2IrO_3 , the itineracy and the non-local correlation are important as well in describing its electronic and magnetic properties due to the extended nature of Ir $5d$ state.

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