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Na_2IrO_3 as a Novel Relativistic Mott Insulator with a 340 meV Gap RICCARDO COMIN, G. LEVY, I. ELFIMOV, A. DAMASCELLI, Quantum Matter Institute, UBC, Vancouver, Canada, D. STRICKER, J. HANCOCK, D. VAN DER MAREL, Université de Genève, Switzerland, Y. SINGH, Indian Institute of Science Education and Research, Mohali, India, P. GEGENWART, Georg-August-Universitat Göttingen, Germany — We have studied Na_2IrO_3 by ARPES, optics, and band structure calculations in the local-density approximation (LDA). The weak dispersion of the Ir $5d$-t_{2g} manifold highlights the importance of structural distortions and spin-orbit coupling (SO) in driving the system closer to a Mott transition. We detected an insulating gap $\Delta_{gap} \simeq 340\,\mathrm{meV}$ which, at variance with a Slater-type description, is already open at 300 K and does not show significant temperature dependence even across $T_N \simeq 15\,\mathrm{K}$. An LDA analysis with the inclusion of SO and Coulomb repulsion U revealed that, while the prodromes of an underlying insulating state are already found in LDA+SO, the correct gap magnitude can only be reproduced by LDA+SO+U, with $U = 3\,\mathrm{eV}$. This establishes Na_2IrO_3 as a novel type of Mott-like correlated insulator in which Coulomb and relativistic effects have to be treated on an equal footing.

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