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Title:	Na ₂ IrO ₃ as a Novel Relativistic Mott Insulator with a 340-meV Gap
Authors:	Singh, Yogesh (/jspui/browse?type=author&value=Singh%2C+Yogesh)
Keywords:	Spin-orbit LDA Spectroscopy
Issue Date:	2013
Publisher:	American Physical Society
Citation:	Physical Review Letters, 109(26).
Abstract:	We study Na ₂ IrO ₃ by angle-resolved photoemission spectroscopy, 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 (SO) coupling in driving the system closer to a Mott transition. We detect an insulating gap Δ gap \approx 340 meV which, at variance with a Slater-type description, is already open at 300 K and does not show significant temperature dependence even across $T_N \approx 15$ K. An LDA analysis with the inclusion of SO and Coulomb repulsion U reveals 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 eV. This establishes Na ₂ IrO ₃ as a novel type of Mott-like correlated insulator in which Coulomb and relativistic effects have to be treated on an equal footing.
Description:	Only IISERM authors are available in the record.
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