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Title:	Na <sub>2</sub> IrO <sub>3</sub> as a novel relativistic mott insulator with a 340-meV gap
Authors:	Singh, Yogesh (/jspui/browse?type=author&value=Singh%2C+Yogesh)
Keywords:	Angle resolved photoemission spectroscopy Band structure calculation
Issue Date:	2012
Publisher:	The American Physical Society
Citation:	Physical Review Letters, 109 (26), Art. No. 266406
Abstract:	We study Na <sub>2</sub> IrO <sub>3</sub> by angle-resolved photoemission spectroscopy, optics, and band structure calculations in the local-density approximation (LDA). The weak dispersion of the Ir 5d-t <sub>2g</sub> 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 $\Delta_{\text{gap}} \approx 340$ 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 <sub>2</sub> IrO <sub>3</sub> 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.
URI:	<a href="http://prl.aps.org/abstract/PRL/v109/i26/e266406">http://prl.aps.org/abstract/PRL/v109/i26/e266406</a> ( <a href="http://prl.aps.org/abstract/PRL/v109/i26/e266406">http://prl.aps.org/abstract/PRL/v109/i26/e266406</a> )
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