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Na2IrO3 by ARPES: a spin-orbit-induced band insulator.

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We study the low-energy electronic structure of the insulating compound Na2IrO3 by angle-resolved photoemission spectroscopy (ARPES) and density functional theory (DFT). Since in DFT calculations within the local density approximation (LDA) this system is metallic, yet with very narrow bands, it has been proposed that Na2IrO3 might be the realization of a Mott insulator in a 5d transition metal oxide. The ARPES experiments were performed both on the pristine cleaved surfaces and as a function of in-situ carrier doping via potassium deposition. From the K-induced chemical potential shift and the emergence of spectral weight across the insulating gap, as well as complementary optical conductivity experiments, we have been able to obtain a precise quantitative estimate of the optical gap Delta=350 meV. By performing detailed LDA calculations, accounting also for spin-orbit interaction (SO) and Coulomb repulsion U, we find that while the correct gap magnitude can only be reproduced in LDA+SO+U calculations, a clear gap is already open everywhere in momentum space simply with the inclusion of spin-orbit (LDA+SO). This establishes Na2IrO3 as a spin-orbit-induced band insulator.

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