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Title:	Chemical tuning between triangular and honeycomb structures in a 5d spin-orbit Mott insulator
Authors:	Mehlawat, K. (/jspui/browse?type=author&value=Mehlawat%2C+K.) Singh, Yogesh (/jspui/browse?type=author&value=Singh%2C+Yogesh)
Keywords:	Structural properties Iridates Mott insulators X-ray diffraction
Issue Date:	2019
Publisher:	American Physical Society
Citation:	Physical Review B, 100(21).
Abstract:	We report structural studies of the spin-orbit Mott insulator family $K_xIr_yO_2$ , with triangular layers of edge-sharing $IrO_6$ octahedra bonded by potassium ions. The potassium content acts as a chemical tuning parameter to control the amount of charge in the Ir-O layers. Unlike the isostructural families with Ir replaced by Co or Rh ( $y=1$ ), which are metallic over a range of potassium compositions $x$ , we instead find insulating behavior with charge neutrality achieved via iridium vacancies, which order in a honeycomb supercell above a critical composition $x_c$ . By performing density functional theory calculations we attribute the observed behavior to a subtle interplay of crystal-field environment, local electronic correlations, and strong spin-orbit interaction at the $Ir^{4+}$ sites, making this structural family a candidate to display Kitaev magnetism in the experimentally unexplored regime that interpolates between triangular and honeycomb structures.
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