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Title: Electronic and structural properties of the honeycomb iridates A2IrO3 (A=Na, Li) at elevated

pressures

Authors: Singh, Yogesh (/jspui/browse?type=author&value=Singh%2C+Yogesh)

Keywords: Honeycomb structures

Electric conductivity
Lithium metallography

X-ray diffraction measurements

Issue Date: 2020

Publisher: American Physical Society

Citation: Physical Review B, 102(8)

Abstract:

The honeycomb lattice iridates A2IrO3 (A=Na, Li) are spin-orbit assisted Mott insulators proximate to Kitaev's quantum spin liquid. The insulating state as well as the magnetic properties are believed to arise due to a delicate balance of several energy scales. We report on high-pressure electrical transport and X-ray-diffraction measurements on A2IrO3 (A=Na, Li) in an attempt to study their structural and electronic evolution with pressure. We found that while Li2IrO3 undergoes a structural phase transition into the dimerized state at a pressure of P ~4 GPa, in Na2IrO3 the conservation of the original C2/m structure up to at least 58 GPa is observed. In addition, Li2IrO3 undergoes a sluggish structural rearrangement at the pressure range 20-40 GPa coinciding with a significant decrease in resistance. Despite dissimilar structural evolution and different mechanisms of the electrical conductivity, Arrhenius conductivity for Na2IrO3 and Mott variable-range hopping in Li2IrO3, both systems show a very similar R(P) behavior. Namely, after a nonmonotonic decrease of the resistance R and the charge gap  $\Delta$ , the  $\Delta$  stabilizes at about 45 GPa and even increases slightly with pressure; the R(T) shows insulating behavior up to the highest pressure measured, 80 and 55 GPa, respectively. This resilient nonmetallic behavior of the studied iridates suggests a formation close to a localized-itinerant crossover of unusual electronic states, whose possible features are discussed. Unforeseeably, the R(P) behavior is not dependent on the buffer element A, which seems essential for understanding the nature of the electrical conductivity in iridates.

Description: Only IISERM authors are available in the record.

URI: https://journals.aps.org/prb/abstract/10.1103/PhysRevB.102.085156

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