Simultaneous Metal-Insulator and Antiferromagnetic Transitions in Orthorhombic Perovskite Iridate Sr0.94Ir0.78O2.68 Single Crystals

H. ZHENG, Department of Physics, University of Colorado, Boulder, CO, J. TERZIC, Center for Advanced Materials and Department of Physics and Astronomy University of Kentucky, KY, F. YE, Quantum Condensed Matter Division, Oak Ridge National Laboratory, TN, X. G. WAN, D. WANG, Department of Physics, Nanjing University, China, J. WANG, Quantum Condensed Matter Division, Oak Ridge National Laboratory, TN, X. P. WANG, Chemical and Engineering Materials Division, Oak Ridge National Laboratory, TN, P. SCHLOTTMANN, Department of Physics, Florida State University, FL, S. J. YUAN, Center for Advanced Materials and Department of Physics and Astronomy University of Kentucky, KY, G. CAO, Department of Physics, University of Colorado, Boulder, CO — We report results of our investigation of bulk single-crystal Sr0.94Ir0.78O2.68 or Ir-deficient, orthorhombic perovskite SrIrO3. It retains the same crystal structure as stoichiometric SrIrO3 but exhibits a sharp, simultaneous antiferromagnetic (AFM) and metal-insulator (MI) transition occurring in the basal-plane resistivity at 185 K. All results including our first-principles calculations underscore a delicacy of the paramagnetic, metallic state in SrIrO3 that is in close proximity to an AFM insulating state.

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