

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Structural phase transition induced by van Hove singularity in 5d transition metal compound IrTe₂ TIAN QIAN, HU MIAO, ZHIJUN WANG, Institute of Physics, Chinese Academy of Sciences, XUERONG LIU, Brookhaven National Laboratory, XUN SHI, YAobo HUANG, PENG ZHANG, NAN XU, PIERRE RICHARD, Institute of Physics, Chinese Academy of Sciences, MING SHI, Paul Scherrer Institute, Swiss Light Source, Switzerland, M.H. UPTON, Advanced Photon Source, Argonne National Laboratory, J.P. HILL, Brookhaven National Laboratory, GANG XU, XI DAI, ZHONG FANG, Institute of Physics, Chinese Academy of Sciences, H.C. LEI, C. PETROVIC, Brookhaven National Laboratory, AIFANG FANG, NANLIN WANG, HONG DING, Institute of Physics, Chinese Academy of Sciences — Comprehensive studies of the electronic states of Ir 5d and Te 5p have been performed to elucidate the origin of the structural phase transition in IrTe₂ by combining angle-resolved photoemission spectroscopy and resonant inelastic X-ray scattering. While no considerable changes are observed in the configuration of the Ir 5d electronic states across the transition, indicating that the Ir 5d orbitals are not involved in the transition, we reveal a van Hove singularity at the Fermi level (E_F) related to the Te $p_x + p_y$ orbitals, which is removed from E_F at low temperatures. The wavevector connecting the adjacent saddle points is consistent with the in-plane projection of the superstructure modulation wavevector. These results can be qualitatively understood with the Rice-Scott “saddle-point” mechanism, while effects of the lattice distortions need to be additionally involved.

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Date submitted: 13 Nov 2013

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