

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Bonding instability induced Surface Insulating State in IrTe₂ A.G.

GIANFRANCESCO, Univ of TN, Knoxville, Q. LI, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, J.Q. YAN, Dept of Materials Science and Engineering, Univ of TN, Knoxville, TN 37996, USA, X. CHEN, Materials Science and Technology Div, ORNL, Oak Ridge, TN 37831, USA, W. LIN, S. KALININ, CNMS, ORNL, Oak Ridge, TN 37831, USA, D.J. SINGH, MSTD, ORNL, Oak Ridge, TN 37831, USA, D. MANDRUS, Dept of MSE, Univ of TN, Knoxville, TN 37996, USA, M. PAN, CNMS, ORNL, Oak Ridge, TN 37831, USA — Using STM/S and DFT calculations, we find that the surface of in-situ cleaved IrTe₂ undergoes a structural transition from trigonal to triclinic lattice below transition temperature, accompanied by formation of unidirectional structural modulations with distinct wavelengths. As temperature approaches 4 K, the system changes into a phase with formation of a single modulated structure with a fully-developed insulating gap. DFT rules out the CDW instability as the origin of this transition, confirming local structural distortion induced orbital degeneracy leading to strong-repulsion between Te p-band, therefore producing an insulating Te surface layer while the bulk stays metallic. This research was conducted (QL, WL, MP) at the CNMS, sponsored at ORNL by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. DOE. Research was supported (WL, SVK) by MSED, Basic Energy Sciences, the U.S. DOE. Fellowship support (AG) from the UT/ORNL Brederesen Center for Interdisciplinary Research and Graduate Education.

Anthony Gianfrancesco
Univ of Tennessee, Knoxville

Date submitted: 15 Nov 2013

Electronic form version 1.4