Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Charge density wave transition in single-layer titanium diselenide
PENG CHEN, University of Illinois at Urbana-Champaign, YANG-HAO CHAN, Academia Sinica, XINYUE FANG, University of Illinois at Urbana-Champaign, YI ZHANG, Nanjing University, MEI-YIN CHOU, Academia Sinica, SUNG-KWAN MO, ZAHID HUSSAIN, ALEXEI FEDOROV, Lawrence Berkeley National Laboratory, TAI-CHANG CHIANG, University of Illinois at Urbana-Champaign — A single molecular layer of titanium diselenide ($TiSe_2$) is a promising material for advanced electronics beyond graphene-a strong focus of current exploration. Such molecular layers are at the quantum limit of device miniaturization and can show enhanced electronic effects not realizable in thick films. We show that single-layer $TiSe_2$ exhibits a charge density wave (CDW) transition at critical temperature T_C =232 K, which is higher than the bulk T_C =200 K. Angle-resolved photoemission spectroscopy measurements reveal a small absolute bandgap at room temperature, which grows wider with decreasing temperature T below T_C in conjunction with the emergence of (2x2) ordering. The results are rationalized in terms of first-principles calculations, symmetry breaking and phonon entropy effects. The observed BCS behaviour of the gap implies a mean-field CDW order in the single layer and an anisotropic CDW order in the bulk.

Peng Chen
Lawrence Berkeley National Laboratory

Date submitted: 03 Nov 2015 Electronic form version 1.4