Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Dirac fermions in monolayer TiB_2 LIZHI ZHANG, SHIXUAN DU, HONGJUN GAO, FENG LIU, The University of Utah — Monolayer TiB_2 sheet (m-TiB_2), a two-dimensional metal-diboride, is investigated by first-principles calculations. We demonstrate that m-TiB_2 maintains isotropic Dirac cones near the Fermi level, having a Fermi velocity about one-half of the Fermi velocity of graphene. Different form graphene, these Dirac cones are located between K and Γ point in the Brillouin zone, and have primarily the transition metal *d-orbit* characters. Further analysis illustrates that the d-band Dirac cones arise from the hybridization of B $p$and Ti d orbitals. Calculations of adsorption of the m-TiB_2 on hexagonal BN (h-BN) substrate reveal a negligible influence of the h-BN substrate to the electronic properties of m-TiB_2. Our findings extend the Dirac-band materials to metal-diborides.

Lizhi Zhang
The University of Utah

Date submitted: 14 Nov 2013 Electronic form version 1.4