Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

**Dirac Semimetal in Three Dimensions** STEVE YOUNG, Makineni Laboratories, Department of Chemistry, University of Pennsylvania, SAAD ZAHEER, JEFFREY TEO[1], CHARLES KANE, EUGENE MELE, Department of Physics and Astronomy, University of Pennsylvania, ANDREW RAPPE, Makineni Laboratories, Department of Chemistry, University of Pennsylvania — In a Dirac semimetal the conduction and valence bands contact at discrete points in the Brillouin zone, dispersing linearly away from these critical points with the low energy physics described by a four band Dirac Hamiltonian. In 2D this situation is realized in graphene in the absence of spin-orbit coupling. 3D Dirac semimetals are predicted to exist at the phase transition between a topological insulator and an ordinary insulator when inversion symmetry is preserved. Here we show that 3D Dirac points can also be protected by crystallographic symmetries in particular space groups and enumerate the criteria necessary to identify these groups. As an example of a Dirac semimetal, we present calculations for $\beta$-Cristobalite $BiO_2$ which exhibits Dirac points at the three symmetry related $X$ points of the FCC Brillouin zone. We find that $\beta$-Cristobalite $BiO_2$ is metastable, so it can be physically realized as a 3D analog to graphene. We provide a systematic approach that includes crystallographic symmetry arguments and physical and chemical considerations to identify other such materials and rule out possible alternatives such as HgTe. This would greatly expand the range of applications that take advantage of properties arising from Dirac points.

Steve Young
University of Pennsylvania

[1]Present Address: Department of Physics, University of Illinois at Urbana-Champaign

Date submitted: 11 Nov 2011 Electronic form version 1.4