Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

**Design a giant 3D quantum spin Hall insulator with double pervoskites**[1] HUI WANG, SHU-TING PI, JEONGWOO KIM, Department of Physics and Astronomy, University of California, Irvine, YIN-KOU WANG, Center of General Education, National Taiwan Normal University, CHI-KEN LU, Department of Physics, National Taiwan Normal University, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine — We propose a new approach to find three-dimensional topological insulators (TIs) in which the spin-orbit coupling (SOC) can more effectively generate a band gap. The band gap of conventional TI such as Bi2Se3 is mainly limited by two factors, the strength of SOC and, from electronic structure perspective, the band gap when SOC is absent. While the former is an atomic property, we find that the latter can be minimized in a generic rock-salt lattice model in which band touching at the Fermi level along with band inversion takes place in the absence of SOC. Thus, giant-gap TIs or TIs comprised of lighter elements are expected. The model applies to a class of double perovskites A2BiXO6 (A = Ca, Sr, Ba; X = Br, I) and the band gap is predicted up to 0.55 eV, much larger than known pristine 3D TIs. Besides, the doped compounds might turn into topological superconductors at low temperature since the Bloch states near the Fermi level are unaltered by the dopant at A-site. First-principle calculations considering realistic surface indicate that the Dirac cones are stabilized if proper termination is chosen. The mechanism is general and may open a new vista for future TI-based electronic devices.

[1]Work at University of California, Irvine was supported by DOE-BES (Grants No. DE-FG02-05ER46237 and No. SC0012670) and NERSC for calculations.

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Date submitted: 11 Nov 2016 Electronic form version 1.4