Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Predicting a new quaternary metal oxide and the study of its structural, electronic, and optical properties by density functional theory
PRANAB SARKER, MUHAMMAD N. HUDA, Department of Physics, University of Texas at Arlington — Our recent theoretical and computational research work of a new quaternary metal oxide $CuBiW_2O_8$ and its electronic properties will be presented. Our density functional theory (DFT) total energy calculation using mineral database of relevant oxides determines the crystal structure of $CuBiW_2O_8$ to be a triclinic structure, which agrees with the experimental result. $CuBiW_2O_8$ has a calculated band gap of 1.43 eV suitable for solar-to-hydrogen conversion technology through photoelectrochemical (PEC) approach. The band structure calculation reveals that $CuBiW_2O_8$ possesses indirect band gap. In addition to this, partial DOS plot calculation demonstrates how Cu 3d plays a major role in band gap reduction and why favorable p-d electron transition is likely although band edges are mostly dominated by d orbital electrons. Finally, we find this material is optically anisotropic.

Pranab Sarker
Department of Physics, University of Texas at Arlington

Date submitted: 15 Nov 2012 Electronic form version 1.4