Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Dimensional Reduction: A design tool for new semiconductor compounds for radiation detection[1] B.W. WESSELS, J.A. PETERS, Z. LIU, Dept. of Materials Science and Engineering, Northwestern University, J. ANDROULAKIS, M.G. KANATZIDIS, Dept. of Chemistry, Northwestern University, H. JIN, A.J. FREEMAN, Dept. of Physics, Northwestern University, Evanston, IL 60208 — To address the need for new wide gap semiconductors for efficient radiation detection, we present a new design tool called *dimensional reduction* (DR). The method is based on reducing the dimensionality of highly dense but low bandgap (<1 eV) compounds to create comparably dense wide bandgap (>1.6 eV) semiconductors without compromises on their mass density. We utilize electronic band structure calculations of bandgap and effective mass to aid in the selection among the wide variety of compounds that can be formed by DR. As a proof of the concept, we report on computational design as well as optical characterization of three such dimensionally reduced materials based on β-HgS, HgSe, and CdTe compounds. These compounds, namely, $Cs_2Hg_6S_7$, $Cs_2Hg_3Se_4$, and $Cs_2Cd_3Te_4$, show great promise as detector materials. Band structure calculations show that they have direct bandgaps of 1.28, 1.97, and 2.35 eV, respectively, in good agreement with experimental values of 1.63, 2.2 and 2.5 eV, respectively. Measured electrical resistivity values of $\sim 10^6$, 10^7, and 10^9 Ω-cm, respectively, are high enough for further evaluation of these materials for hard radiation detection. Computational design of other wide gap semiconductors is underway.

[1]This work is supported by the Defense Threat Reduction Agency through grant no. HDTRA1 09-1-0044.

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Date submitted: 17 Nov 2011 Electronic form version 1.4