Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

First principles studies of the stability and Shottky barriers of metal/CdTe(111) interfaces ZHEN LIU, Department of Physics, California State University Northridge, MASOEHNG MIAO, Department of Chemistry and Biochemistry, California State University Northridge, NICHOLAS KIOUSSIS, Department of Physics, California State University Northridge, FIKRI AQARIDEN, Y. CHANG, CHRISTOPH GREIN, Sivananthan Laboratories, 590 Territorial Dr, Unit H Bolingbrook — CdZnTe and CdTe based semiconductor X-Ray and Gamma-Ray detectors have been intensively studied recently due to their promising potentials for achieving high-resolution, high signal-to-noise ratios and low leakage current, all are desirable features in applications ranging from medical diagnostics to homeland security. Using density functional calculations, we systematically studied the stability, the atomic and electronic structures of the interfaces between CdTe (111) surfaces (Cd- and Te-terminated) and the selected metals (Cu, Al Ni, Pd and Pt). We also calculated the Schottky barrier height (SBH) by aligning the electrostatic potentials in semiconductor and metal regions. Our calculations revealed significant differences between the Cd- and Te- terminated interfaces. While metals tend to deposit directly on reconstructed Te-terminated surfaces, they form a Te-metal alloy layer at the Cd-Terminated metal/CdTe interface. For both Te- and Cd- terminated interfaces, the Schottky barrier heights do not depend much on the choice of metals despite the large variation of the work functions. On the other hand, the interface structure is found to have large effect on the SBH, which is attributed to the metal induced states in the gap.

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Date submitted: 06 Nov 2015 Electronic form version 1.4