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First principles studies of the stability and Shottky barriers of metal/CdTe(111) interfaces ODKHUU DORJ, M.S. MIAO, N. KIOUSSIS, California State University Northridge, S. TARI, F. AQARIDEN, Y. CHANG, Sivananthan Laboratories, C. GREIN, University of Illinois at Chicago — 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. Understanding the atomic and electronic structures of the metal/semiconductor interfaces is essential for the further improvements of performance. Using density functional calculations, we systematically studied the stability, the atomic and electronic structures of the interfaces between Cd-terminated CdTe (111) surface and the selected metals. We also calculated the Schottky barrier height (SBH) by aligning the electrostatic potentials in semiconductor and metal regions. Our calculations revealed the importance of intermixing between semiconductor and metal layers and the formation of Te-metal alloys at the interface. The obtained SBH does 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 to the SBH, which is attributed to the metal induced states in the gap. The position of such states is insensitive to the metal work functions, as revealed by the analysis of the electronic structures.

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