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Ohmic contact formation assisted by metallic states at the interface of Cu2Te/CdTe[1] JIN-HO CHOI, RUILONG YANG, WENGUANG ZHU, DELIANG WANG, University of Science and Technology of China, KAI-MING HO, Iowa State University & University of Science and Technology of China, ZHENYU ZHANG, University of Science and Technology of China — Ohmic contact to CdTe is a formidable task, but is indispensable for achieving high-efficiency in CdTe thin film solar cells. Using first-principles calculations within density functional theory, we study the structures and Schottky barrier heights (SBHs) of the widely used Cu_2Te/CdTe contact interfaces. We obtain two main structural configurations of the Cu_2Te layers on CdTe(111), with physically reasonable formation energies: epitaxial and bulk-like Cu_2Te layers. The epitaxial Cu_2Te layers possess Cu-Te bonds with the CdTe(111) surface, maintaining the hexagonal, unreconstructed CdTe(111) structure. In contrast, for the bulk-like Cu_2Te layered, both unreconstructed and reconstructed CdTe(111) surfaces are possible due to weak interactions between the Cu_2Te and CdTe interfaces. Detailed calculations of the SBHs at the Cu_2Te/CdTe interfaces show that the interfaces with an unreconstructed CdTe(111) surface have a low SBH of <0.24 eV, consistent with our experimental observation of <0.3 eV. These findings may serve as an important guidance in future efforts for improving contact quality of semiconductor devices.

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