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Supplementary Information

Interfacial Properties of CdTe-Metal Contacts for Solar Cells

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Supplementary Results and Discussions

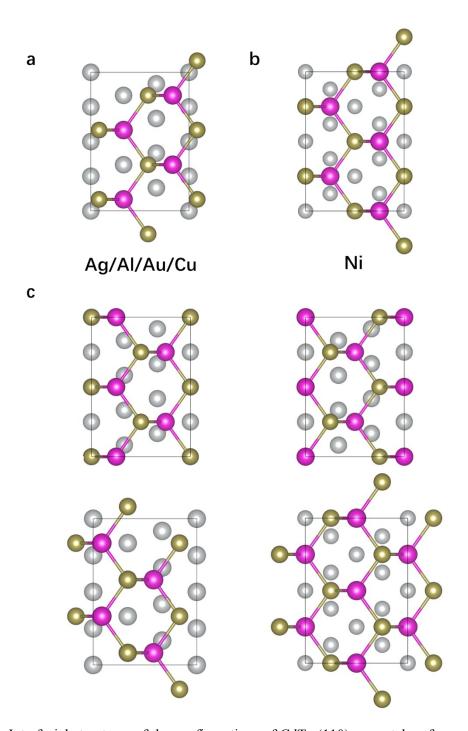


Fig. S1. Interfacial structures of the configurations of CdTe (110) on metal surfaces. (a) Top view of the most stable configuration of CdTe-Ag/Al/Au/Cu surface. (b) Top view of the most stable configuration of CdTe-Ni surface. (c) other configurations we considered.

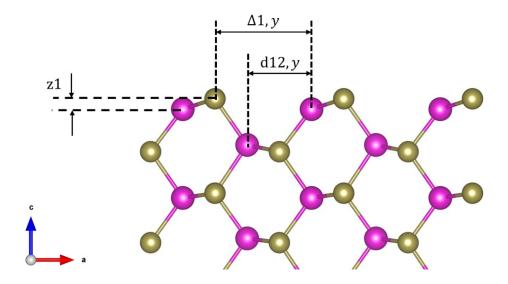


Fig. S2. Side view of the surface geometry of CdTe(110) surface.

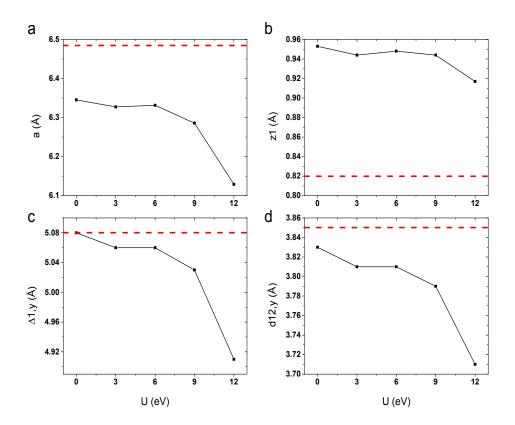


Fig. S3. Test for different values of U. (a) calculated lattice parameter a. (b) calculated z1. (c) calculated $\Delta 1_y$. (d) calculated d12, y. The red dash is the result from LEED.