

## Supporting Information

### Band Alignment for Rectification and Tunneling Effects in Al<sub>2</sub>O<sub>3</sub> Atomic-Layer-Deposited on Back Contact for CdTe Solar Cell

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#### The procedure details for fabrication of CdTe solar cells.

CdTe solar cells were fabricated as following: 200 nm thick CdS window layers were grown on SnO<sub>2</sub>:F/soda-lime (FTO) glass substrate under 300°C by radio frequency magnetron sputtering using a 4N purity (99.99%) target. The substrate were cleaned by sonication in DI water, acetone and isopropanol successively before the deposition of CdS. After CdS, 4-5 μm CdTe absorber layer was deposited by close space sublimation (CSS) under 550°C and Ar with 15% O<sub>2</sub> condition for 20-30 minutes, and the CdTe sources is under 650 °C using 99.999% pure CdTe powder(Alfa Aesar). CdCl<sub>2</sub> thermal treatment was performed following the CdTe deposition. The CdS/CdTe film was first soaked in a 70%-saturated CdCl<sub>2</sub> in methanol solution. The pieces were soaked for 15 min on a hot plate near the boiling point (60-70 °C), then thermal treated under 400 °C for 30minutes in muffle furnace. The CdTe films have a cubic structure and exhibit a strong preferred orientation along the (111) planes parallel to the substrate. The cells were etched in phosphoric acid: nitric-acid: DI-water (NP) to provide a clean, Te-rich surface and then evaporating 3 nm Cu, 150 °C annealing 30 min under N<sub>2</sub> atmosphere to form Cu<sub>x</sub>Te (x=1.44~1) intermediate layer.<sup>1</sup> The CdTe sample was transferred into the ALD system for ultrathin Al<sub>2</sub>O<sub>3</sub> deposition. The ALD system is a custom-built, hot-wall stainless steel cylindrical chamber. Ultrahigh purity nitrogen was used as a purge/carrier gas. Al<sub>2</sub>O<sub>3</sub> was grown using Al(CH<sub>3</sub>)<sub>3</sub>

(TMA), with water as the oxidant. The substrates were maintained at 120 °C throughout the deposition of Al<sub>2</sub>O<sub>3</sub>. The substrate temperature was monitored with a reference thermocouple in the ALD chamber that was previously calibrated against an instrumented wafer. Each cycle of Al<sub>2</sub>O<sub>3</sub> growth consisted of a 1 s dose of TMA, a 25 s purge of N<sub>2</sub>, a 1 s dose of H<sub>2</sub>O, and a 25 s purge of N<sub>2</sub>. The cell was scribed to 0.5 × 0.5 cm<sup>2</sup> area.

**References:**

1. Dzhafarov, T. D.; Yesilkaya, S. S.; Canli, N. Y.; Caliskan, M. Diffusion and Influence of Cu on Properties of CdTe Thin Films and CdTe/CdS Cells. *Sol. Energy Mater. Sol. Cells* **2005**, 85, 371-383.