Supplementary Material (ESI) for Journal of Materials Chemistry

Supporting Information
Atomic Layer Deposition of $Cd_xZn_{1-x}S$ Films

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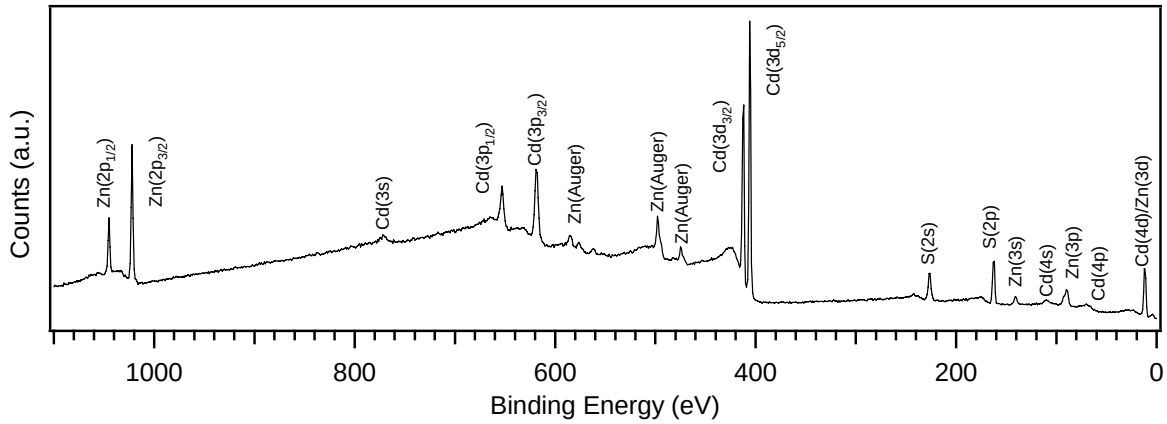

Figure S1: XPS spectrum of a 500 cycle 40% 2x3 alloy deposited at 150 °C on Si(100) shows the presence of only Cd, Zn, and S

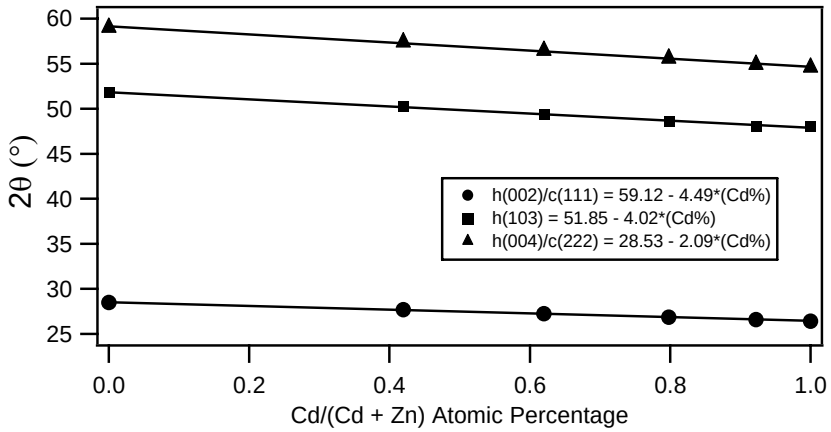

Figure S2: Location of peaks in XRD patterns from Figure 4 as a function of alloy composition as determined by XPS for films deposited at 150 °C on Si(100). The peaks for a given phase are linearly correlated to the composition.

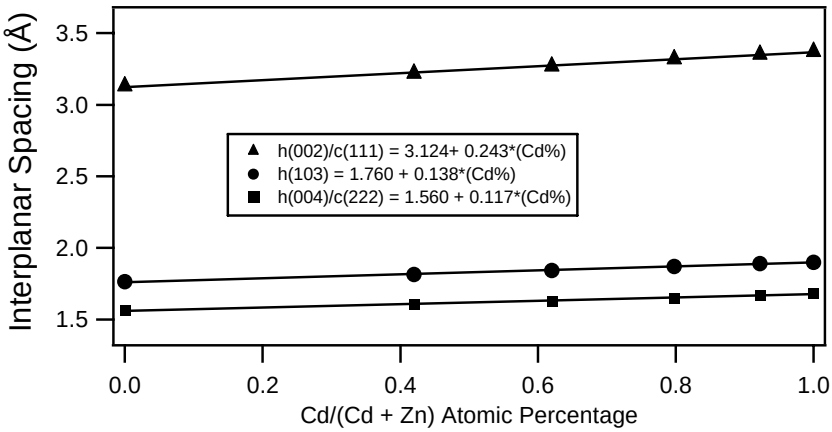

Figure S3: Interplanar spacing as calculated using the XRD patterns in Figure 4 and angles in Figure S2 as a function of alloy composition using Bragg's Law for films deposited at 150 °C. Alloy compositions were determined by XPS

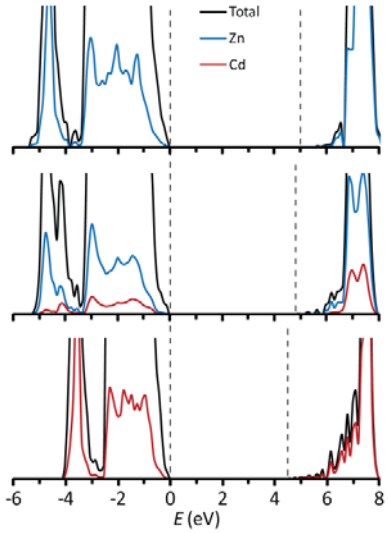

Figure S4: PBE0-calculated electronic density of states of pure ZnS (top), of an alloy with a CdS/(CdS+ZnS) ratio of 0.22 (middle), and of pure CdS (bottom). Top of the valence band is given as zero energy and illustrated, and the dashed lines represent the maximum of valence band and the minimum of conduction band.