Electronic supplementary information for

Room-Temperature Fabrication of a Delafossite $CuCrO_2$ Hole Transport Layer for Perovskite Solar Cells

Wiley A. Dunlap-Shohl,[a] Trey B. Daunis,[b] Xiaoming Wang,[c,d] Jian Wang,[b,e] Boya Zhang,[b] Diego Barrera,[b] Yanfa Yan,[c,d] Julia W. P. Hsu,[b] David B. Mitzi[a,f]

[a] Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC, USA.
[b] Department of Materials Science and Engineering, The University of Texas at Dallas, Richardson, TX, USA.
[c] Department of Physics and Astronomy, The University of Toledo, Toledo, OH, USA.
[d] Wright Center for Photovoltaic Innovation and Commercialization, The University of Toledo, Toledo, OH, USA.
[e] Department of Chemistry, The University of Washington, Seattle, WA, USA.
[f] Department of Chemistry, Duke University, Durham, NC, USA.

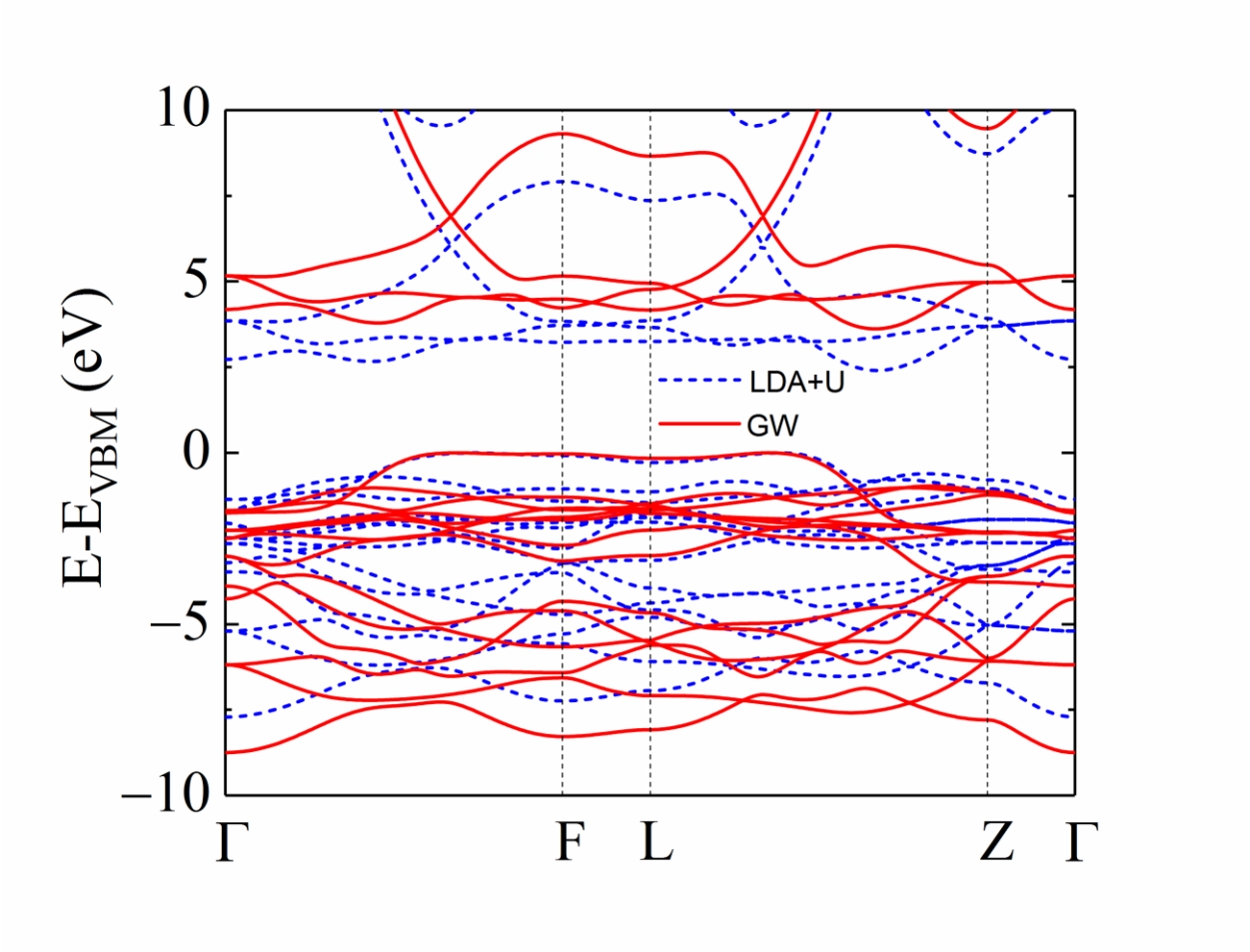

Figure S1. Comparison of the band structures of the 3R CCO in rhombohedral representation calculated by GW and LDA+U. Only the majority spin is shown for clarity.

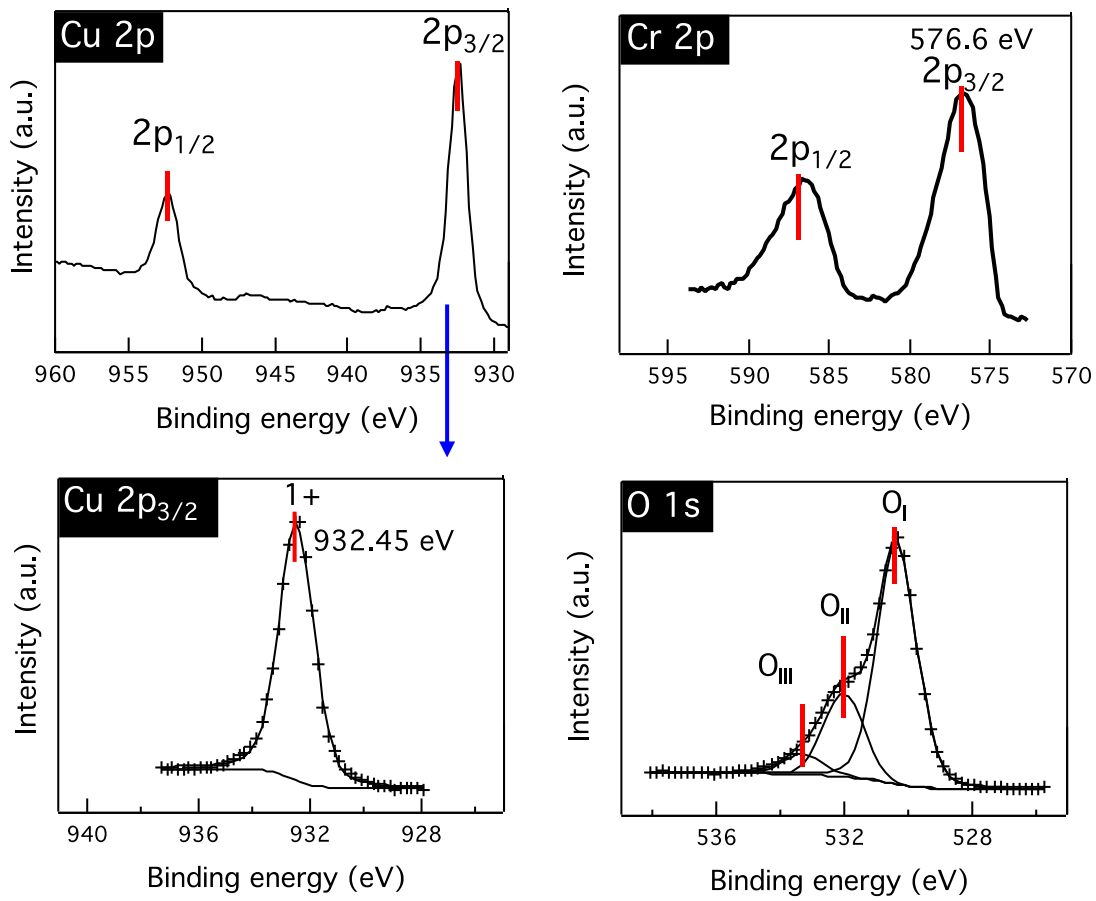

Figure S2. Region scans of X-ray photoelectron spectra of $CuCrO_2$ nanoparticles, demonstrating that the Cu and Cr exist only in mono- and trivalent oxidation states, in accordance with the nominal chemical formula of the material. The XPS analysis using commercial software (Multipak, Ulvac-PHI) reveals a Cu:Cr ratio of 0.9:1.

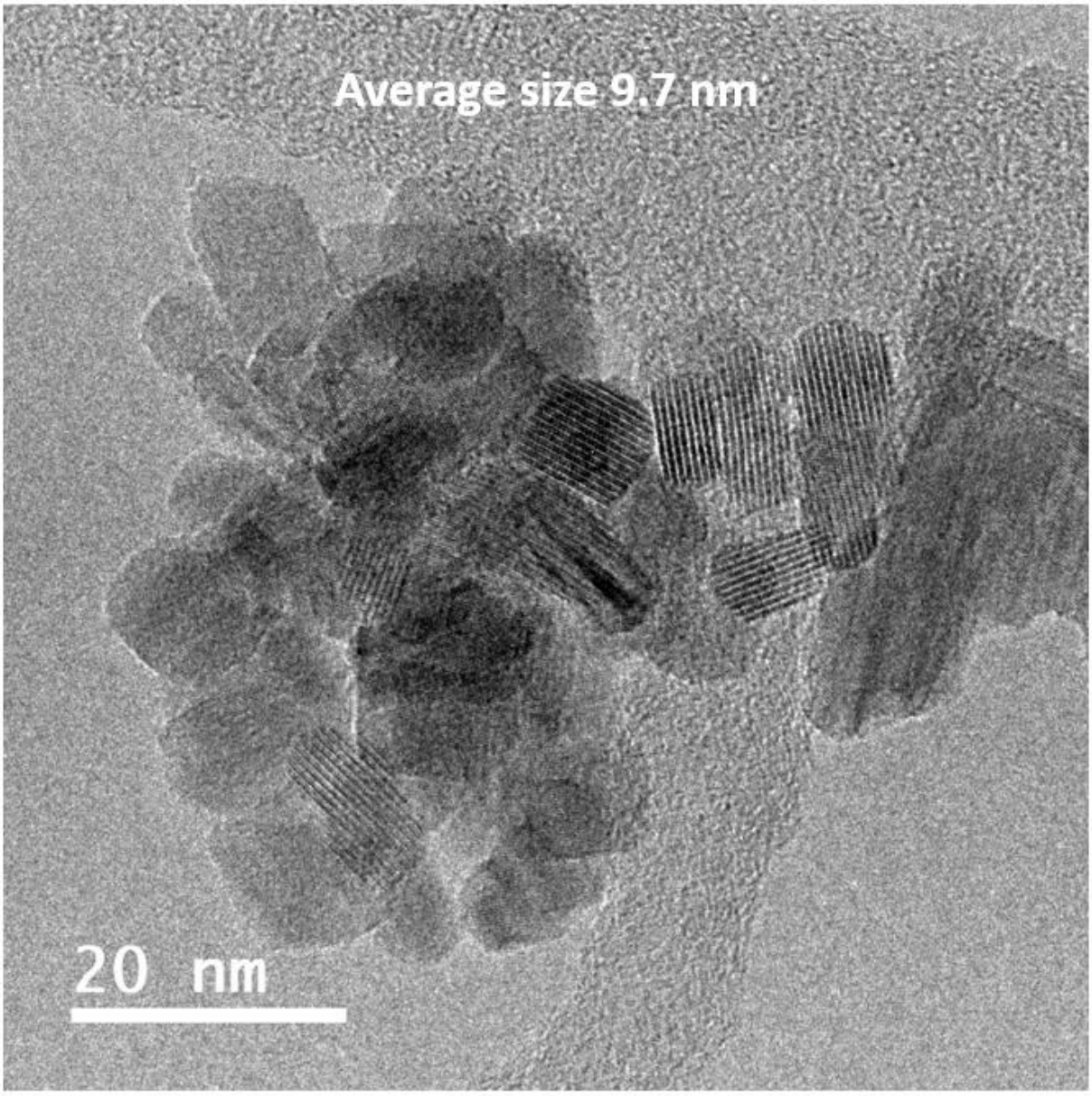

Figure S3. TEM image of CCO nanoparticles, demonstrating roughly isotropic shape and ~10 nm size.

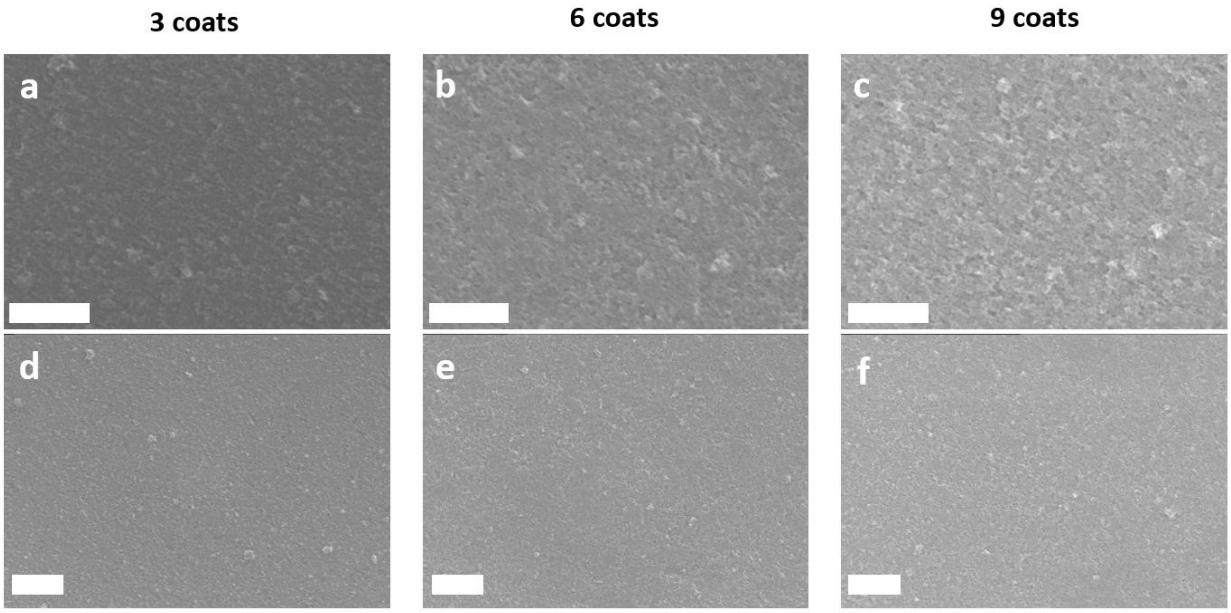

Figure S4. SEM images of CCO films on ITO, demonstrating conformal coverage of the substrate. Scale bars for high-magnification images (a-c): 500 nm; scale bars for low magnification images (d-f): 1 μm.

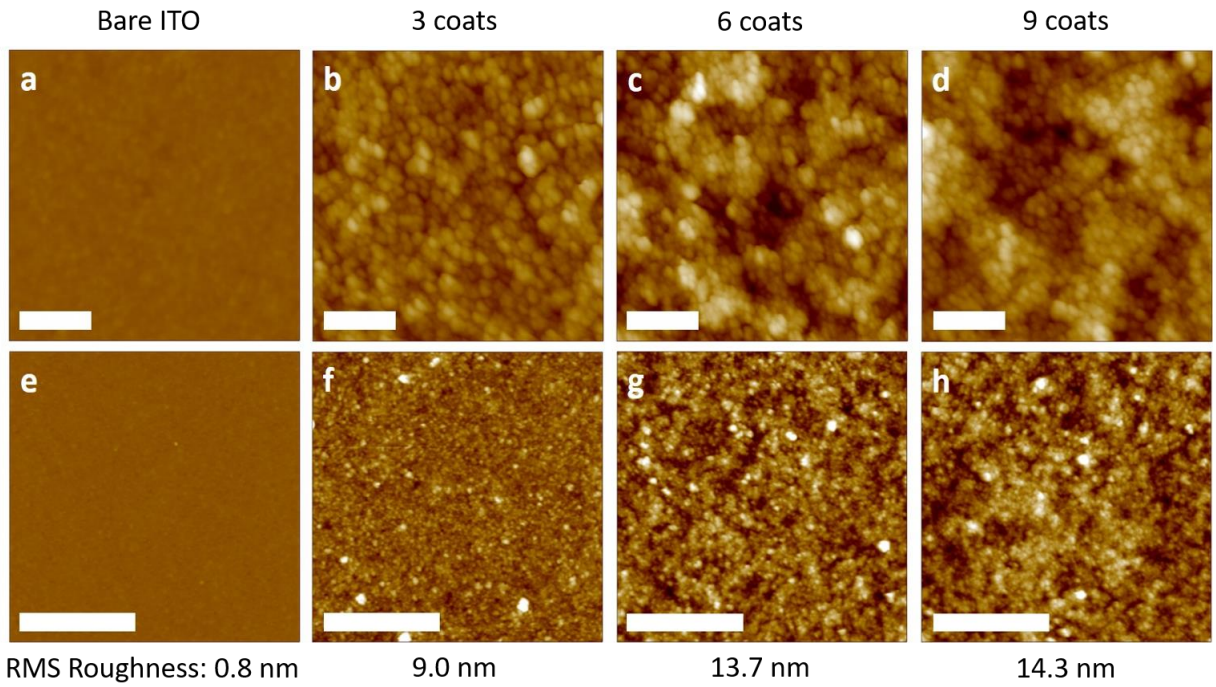

Figure S5. AFM images of CCO films on ITO along with the corresponding RMS roughness values, again demonstrating conformal coverage of the substrate. Scale bars for small area images (a-d): 250 nm; scale bars for large area images (e-h): 2 μm. Color scale for all images is 110 nm. The film RMS roughness values were calculated from 5 μm x 5 μm images.

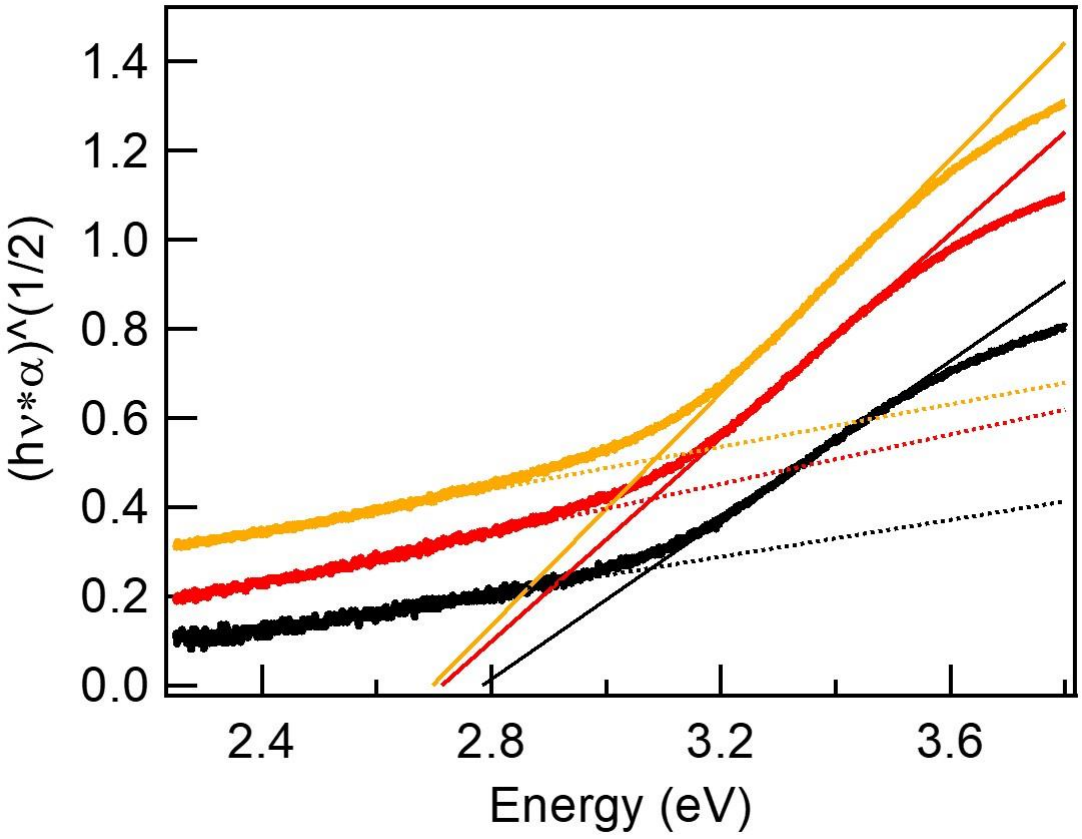

Figure S6. Tauc plots (indirect band gap) of CCO films of several thicknesses (black – 15 nm; red – 30 nm; yellow – 45 nm), showing an indirect transition at ~3.1 eV.

Table S1: Average device parameters at various CCO thicknesses from forward (reverse) J-V scans, using a measurement delay time of 1 s. Uncertainty is represented by the standard deviation of the measurements. 19, 10, 5, 13, 30, 13, and 21 devices were measured for each respective thickness, in ascending order.

CCO Thickness	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
15 nm	0.934 ± 0.022 (0.937 ± 0.029)	20.2 ± 0.3 (20.1 ± 0.3)	57.1 ± 5.4 (56.4 ± 6.5)	10.8 ± 1.2 (10.6 ± 1.4)
17 nm	0.937 ± 0.008 (0.950 ± 0.008)	19.5 ± 0.5 (19.1 ± 0.5)	62.6 ± 1.6 (64.9 ± 1.5)	11.5 ± 0.4 (11.8 ± 0.3)
21 nm	0.963 ± 0.027 (0.975 ± 0.027)	18.8 ± 0.8 (18.6 ± 0.8)	65.6 ± 2.4 (67.1 ± 3.4)	11.8 ± 0.5 (12.1 ± 0.5)
23 nm	0.920 ± 0.010 (0.935 ± 0.017)	20.0 ± 0.3 (19.7 ± 0.2)	69.5 ± 3.1 (69.2 ± 2.9)	12.8 ± 0.6 (12.7 ± 0.6)
30 nm	0.926 ± 0.016 (0.935 ± 0.023)	19.7 ± 0.5 (19.1 ± 0.7)	65.7 ± 3.1 (67.0 ± 3.0)	12.0 ± 0.7 (12.0 ± 0.7)
33 nm	0.917 ± 0.022 (0.927 ± 0.015)	18.7 ± 0.8 (17.5 ± 1.0)	64.4 ± 2.2 (68.2 ± 1.6)	11.0 ± 0.5 (11.0 ± 0.5)
45 nm	0.928 ± 0.015 (0.932 ± 0.025)	19.0 ± 0.4 (18.2 ± 0.5)	60.2 ± 2.9 (63.2 ± 3.5)	10.6 ± 0.6 (10.7 ± 0.7)