Supporting Information: Quantum Efficiency and Bandgap Analysis for Combinatorial Photovoltaics: Sorting Activity of Cu–O Compounds in All-Oxide Device Libraries

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Table S1. PLD deposition parameters for absorber on glass and in device.

sample_name	120626a	120618e
sample_id	609	576
Substrate	glass	TEC7
materials	CuO	TiO2|CuO
layer_id	1077	1177
material	CuO	CuO
sub_layer	1284	1391
Target sample distance (mm) (97+40-82)	55	55
beam_scanner (cm)	51	51
repetition_rate (Hz)	8	8
rastering_vel (mm s^{-1})	29	29
target_vel (mm s^{-1})	29	29
rastering_angle_from (deg)	145	145
rastering_angle_to (deg)	180	180
substrat_vel (mm s^{-1})	0	0
substrat_pos (deg)	0	0
Gas	0	0
MKS (sccm)	5	5
gas_pressure (mTorr)	0.00291	0.00301
Temperature (°C)	23	23
ramp_rate_inc (deg min^{-1})	1	1
ramp_rate_dec (deg min^{-1})	1	1
post_ann_temp (°C)	23	23
post_ann_time (min)	1	1
laser_voltage (kV)	22	22
laser_energy_fluence (mJ)	191	167
laser_power (W)	0.96	0.83
laser_pressure (mBar)	3334	3293
laser_energy_fluence_messured (mJ)	100	100.8
pulses	45000	45000
pulses_cycles	1	1
layer_number	1	2
id	366	383
remarks		TiO2

In order to obtain the TiO_2 monochromatic absorption coefficient, two additional partial libraries were sprayed with TiO_2 on TEC7, under the same routine as that used for this work. The libraries were scanned with the optical scanner and analyzed for absorptance. TEC7 was scanned separately, and the FTO + 2.2 mm glass absorptance was calculated. The TiO_2 absorptance was calculated. The libraries were taken to cross section focused ion beam (FIB), and the FTO and TiO2 layers thickness were measured several times for several locations along a line in the libraries. From the TiO2 absorptance values and the measured thickness, the absorption coefficient was calculated.

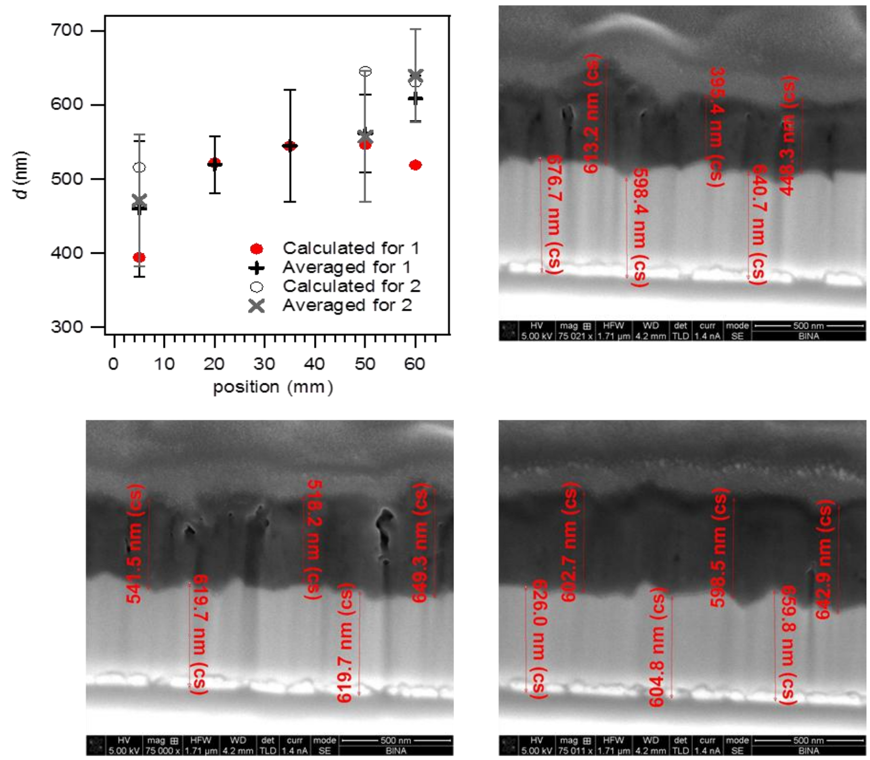

Figure S1. In order to obtain the Cu_xO thickness, profilometer measurements were taken on the PLD deposition shoulder. The thickness profile of the entire library was obtained with eq. **Error! Reference source not found.**, as explained in the Cu_xO thickness section.

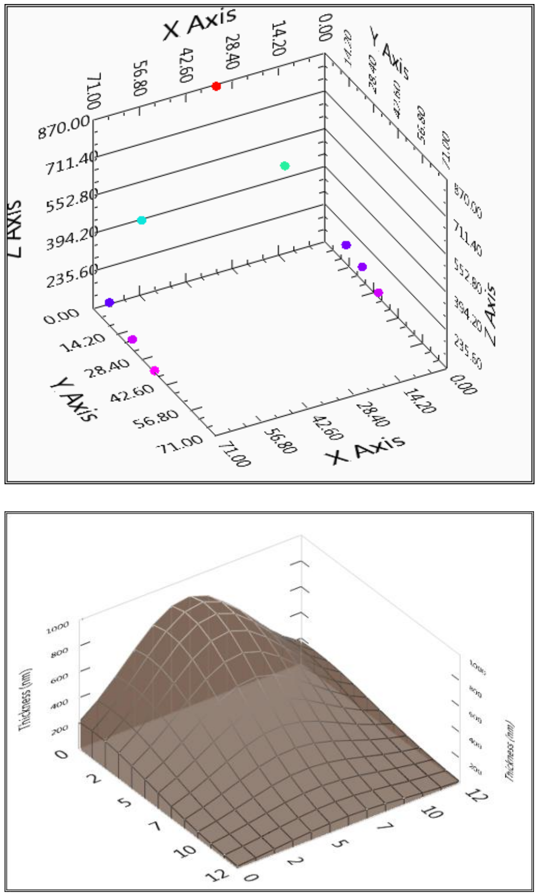

Figure S2. Top - Profilomter measurements of the deposited Cu_xO layer on glass. Bottom – the solution of the deposition profile after fitting eq 2 for each index in the library.

Table S2. Fitting parameters for the thickness of the Cu_xO using eq. 2.

Ny	11.69 mm
Ay	889.57 nm
hy	6.43 mm
Nx	20.36 mm
hx	33.90 mm
H	55.00 mm

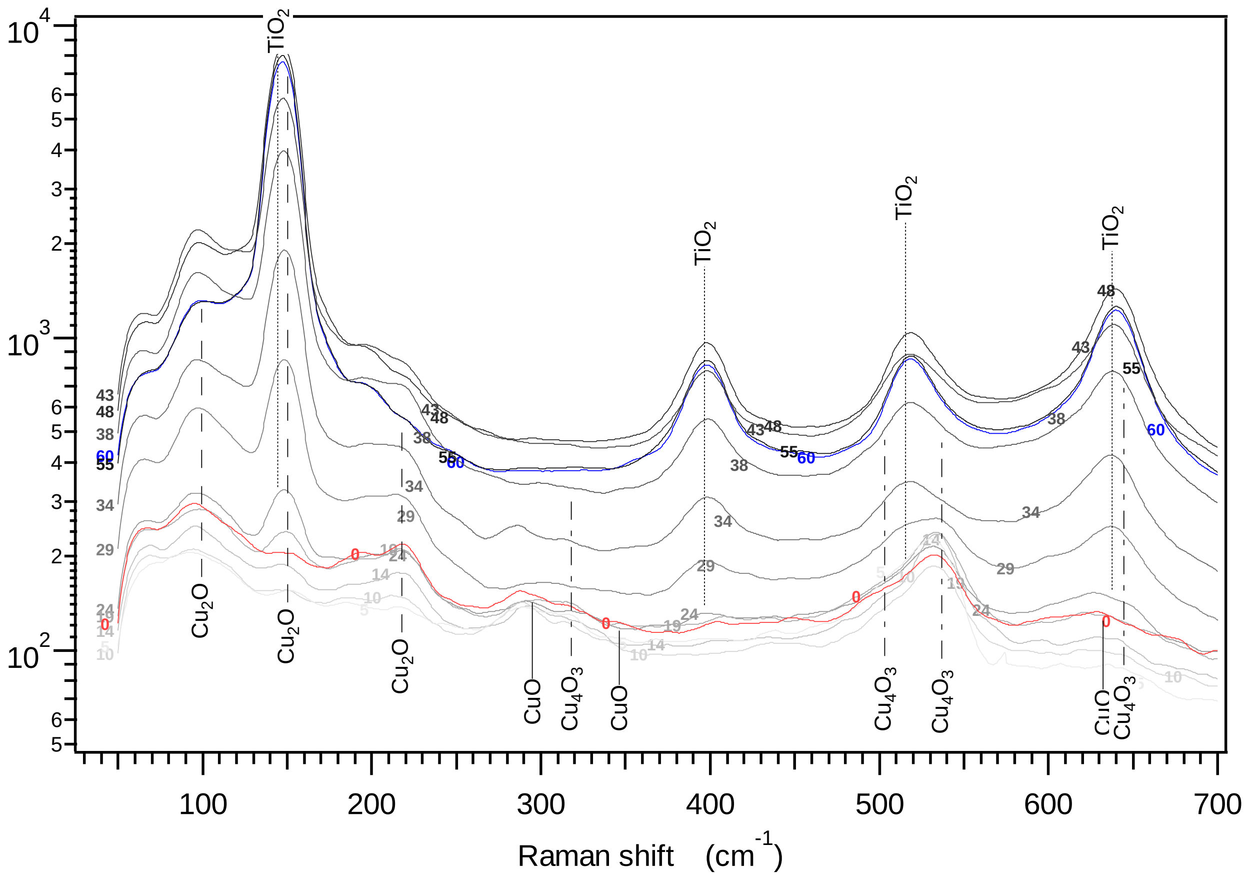

Figure S3. Raman spectra with peak allocation to CuO, Cu_4O_3 Cu_2O and TiO_2 presented with logarithmic non-offset counts scale.

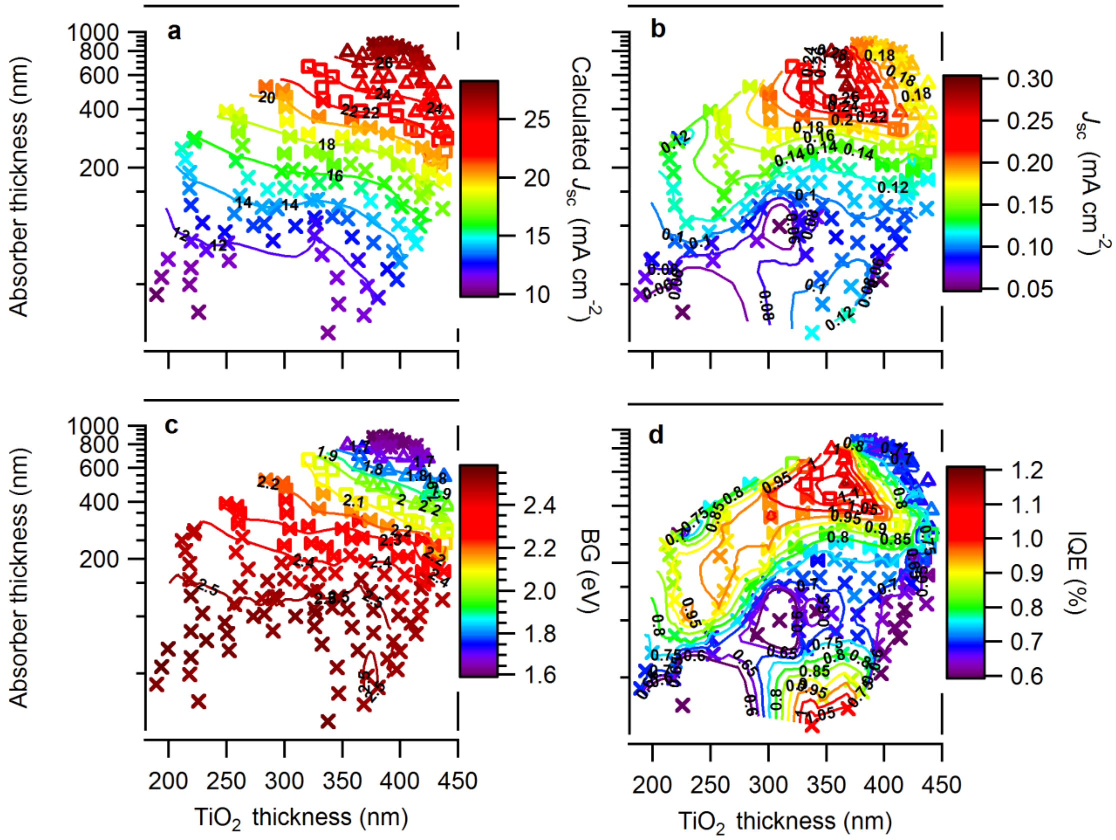

Figure S4. (**a**) Plot of maximum theoretical short circuit photocurrent (J_{calc}) as a function of TiO_2 and Cu-O layer thicknesses, with logarithmic absorber thickness scale. (**b**) Plot of short circuit photocurrent (J_{sc}) as a function of layer thicknesses, with logarithmic absorber thickness scale. (**c**) Plot of fitted bandgaps (BG) as a function of layer thicknesses, with logarithmic absorber thickness scale. (**d**) Plot of calculated Internal Quantum Efficiency (IQE) as a function of layer thicknesses, with logarithmic absorber thickness scale.

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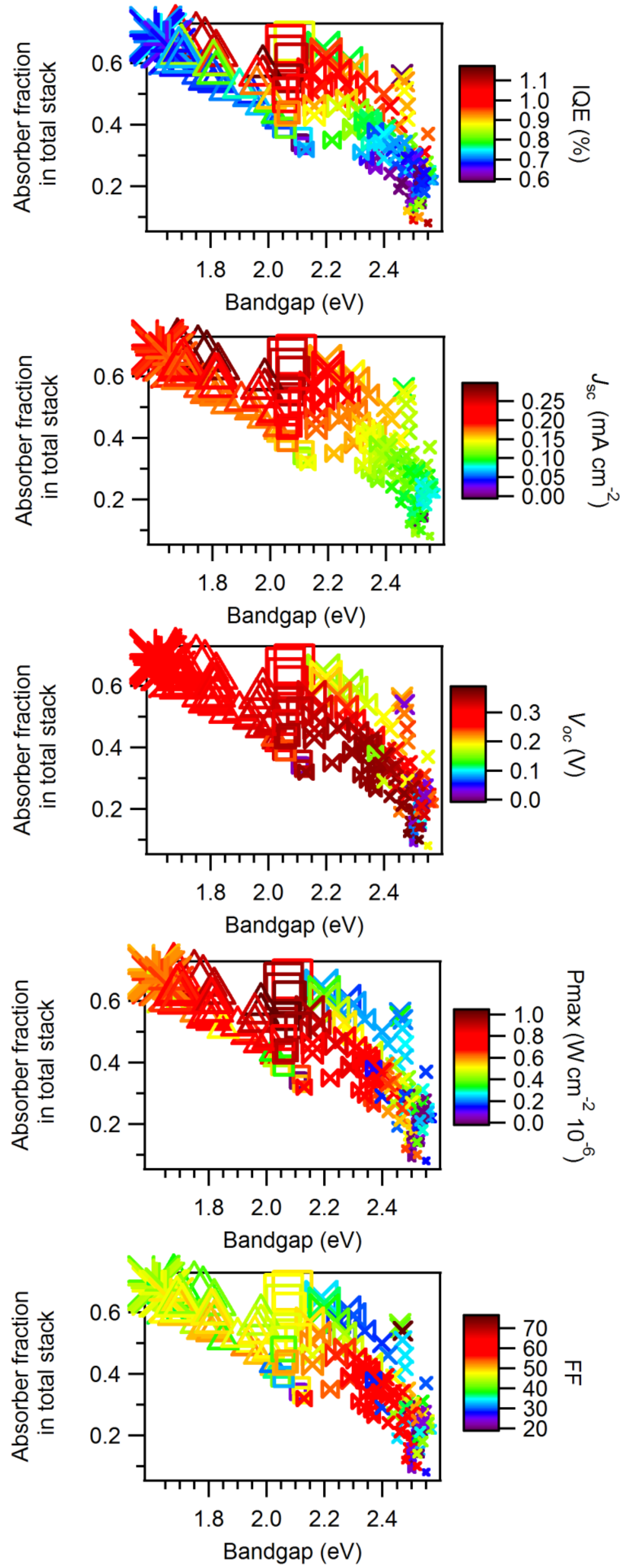

Figure S5. Internal quantum efficiency (IQE), short circuit photocurrent (J_{sc}), Open circuit Photovoltage (V_{oc}), maximum power (Pmax) and Fill Factor (FF), plotted as a function of absorber fraction in total stack and bandgap. The sizes of the symbols correlate with the absorber thickness.