Supporting Information

Colorimetric screening for high-throughput discovery of light absorbers

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Photo-scanning and colorimetric algorithm

We use the following procedure on both transparent (2.2 millimeter thick glass plates with a 400 nm coating of transparent conductive oxide TEC15), and opaque substrates (silicon wafers, stainless steel and nickel plates). All substrates are scanned in reflection mode (EPSON Perfection V600), and the transparent substrates are also scanned in transmission (EPSON Perfection V750). In Fig. S1(a) we have five bandpass filters scanned and their wavelength is compared to the hue value obtained from the photo-scanned images (also in the figure). The Xe lamp source in V750 and the LED light source in V600 are expected to deteriorate in performance with time, so in order to have reproducible and comparable results, we use a common standard used by photographers, known as the Macbeth color chart (here, ColorChecker Classic by X-rite Photo), as shown in Fig. S1(b). The results that we expect from our colorimetric screen on the color chart are represented in Fig. S1(c). Any high-throughput color screening protocol should include this color check as a part of the process.

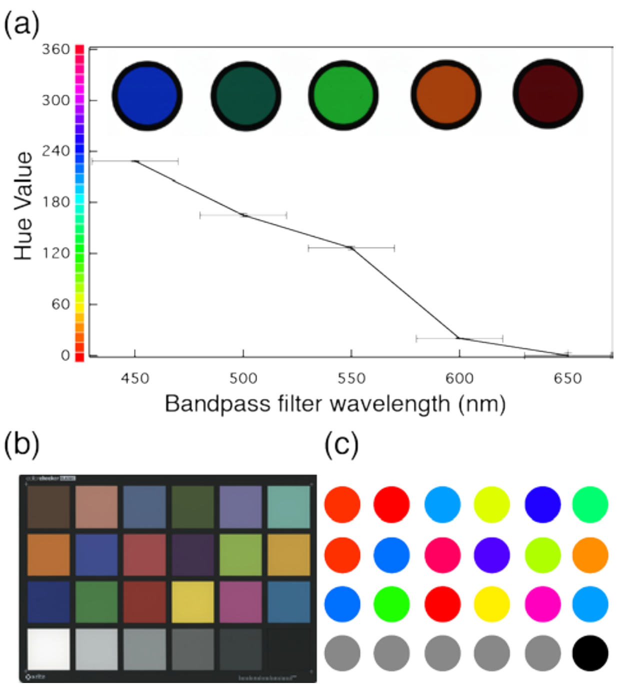

Figure S1. (a) Relationship of the hue registered by the photoscanner to the wavelength of bandpass filters. The actual photoscans of the five bandpass filters (ThorLabs) are in the image above the graph. (b) Photoscan of the Macbeth color standard chart. (c) The values of the hue from the sections of the Macbeth chart in Fig. S1(b). Same color scale is used as in Fig. 1 of the Technical Note.

The hue value, and the relationship of brightness and saturation to describe the full HSB color space are presented in Fig. S2(a). Fig. S2(b) shows the color space of a single hue value, and illustrates how we choose to assign the gray (G) and black (B) values. The thresholds in dashed yellow lines are parameters in the code, and for the examples in the paper, they are chosen to be 10% and 20%, respectively. White (W) pixels are only in special cases actually close to white – meaning highest brightness at lowest saturation. This would be the case for glass plates which transmit light well enough to get the reflection from the white backing of the photoscanner lid. The substrate may appear as grey (metallic substrates) or black (for silicon).

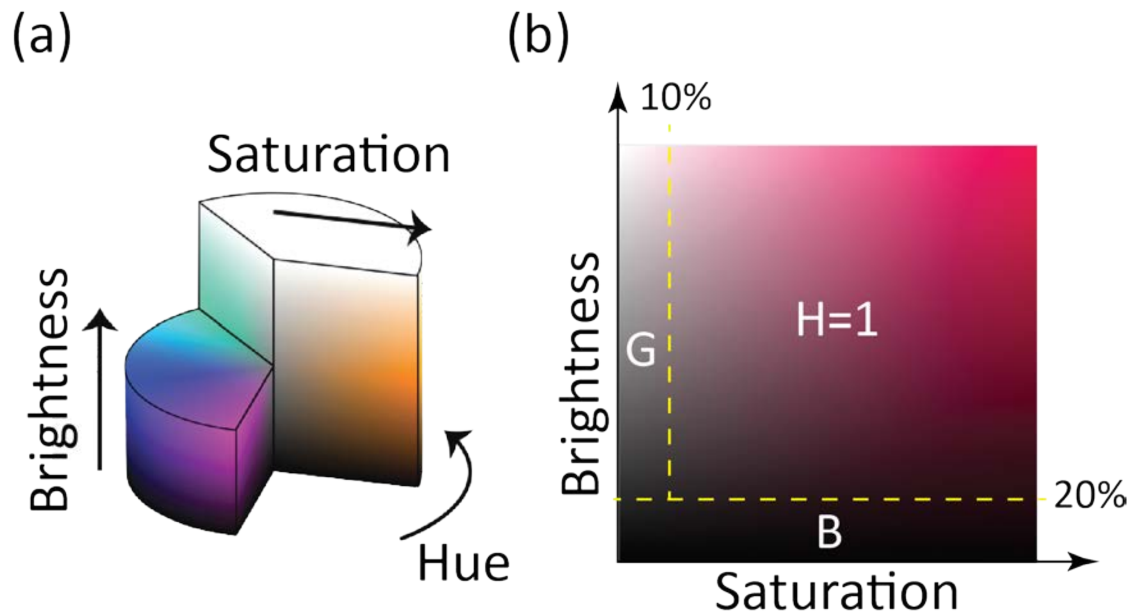

Figure S2. (a) The HSB color space. (Adapted from an image available on Wikipedia.org, By Jacob Rus, Under Creative Commons license CC BY-SA 3.0). (b) The HSB space of a single hue value (H=1 in this case). The yellow lines illustrate the thresholds for gray and black pixels.

The substrates with sample Spots are photoscanned, and then go through Metrology procedure, whose purpose is to identify the Spots on the substrate and align them with a predefined grid of samples (see Figure S3). This is used to identify and locate individual sample Spots, to automate further measurements in our screening instruments, including UV-Vis scanners. Once the sample locations are identified, the image is cropped into 51 x 51 pixel images of individual Spots (dashed outline in Figure 1(a), and blue squares in Fig. S3). The colorimetric algorithm runs on these images, individually, or in parallel with algorithm parallelization. The process of cropping and running colorimetric algorithm is automatic, and the results appear in the database viewer assembled into compositional spaces.

Colorimetric algorithm reads the RGB value for each pixel in the image and recalculates the values into the HSB space using transformation routines built into the Magick++ API. Pixels are then sorted into categories, based on the threshold parameters. In Fig. S2(b) we illustrate how the choice is made when selecting brightness and saturation thresholds. A histogram is created for each spot (Fig. 1(a)) containing designated W, G, B pixels and hues into 32 bins. The hue range is then analyzed for the most contributing bin, and the bins around it are counted under that same bin value. Depending on the

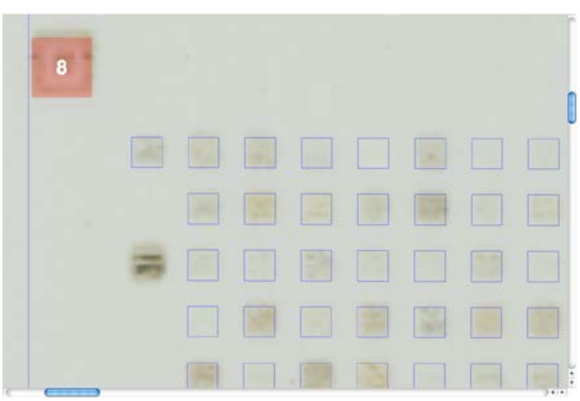

Figure S3. Screenshot of the Metrology application. Computer identifies fiducial markers and aligns the grid of sample positions corresponding to a known sample map used to print samples. The user then makes adjustments until all samples fall into the grid (blue squares). The grid is then used to automatically crop the large image into images of individual sample Spots.

magnitude of the bins around, this may include more than just the nearest neighbor binds. The histogram is then used to make a pie chart as explained in the Technical Note and in Fig. 1.

Results from a quaternary library of Bi-Mn-V-Ce oxides

In Figure S4 the cropped Spots from the photoscan of the plate library (Figure 3(a)) are assembled into quasi-ternary cuts along the increasing Ce composition direction. The nominal concentration step is 5%. In Figure S5 we show the corresponding color screen result, and in Figure S6 the result of the direct allowed bandgap from Tauc plot analysis.

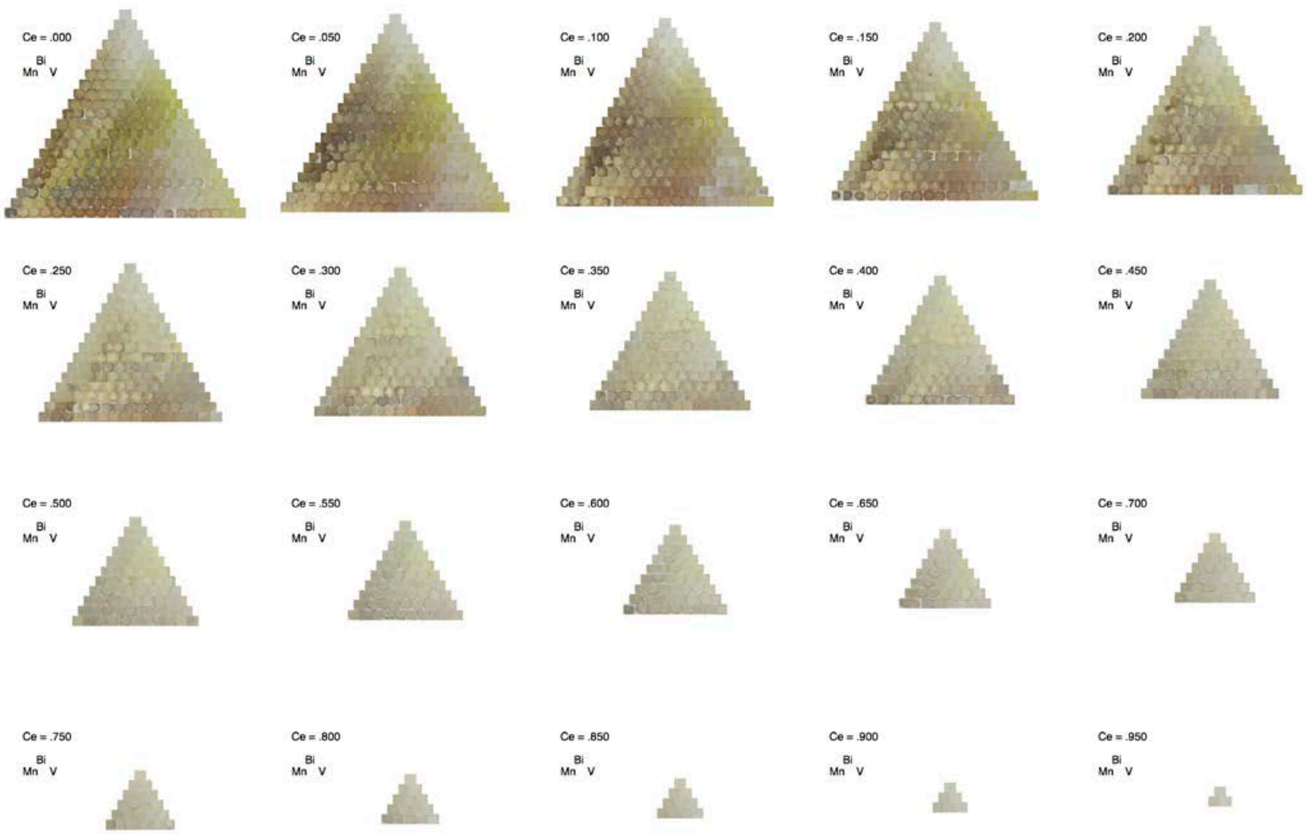

Figure S4. Photoscanned images of plate in Figure 3(a) assembled into quasi-ternary compositional spaces, which can be stacked on top of each other to create a full quaternary space tetrahedron.

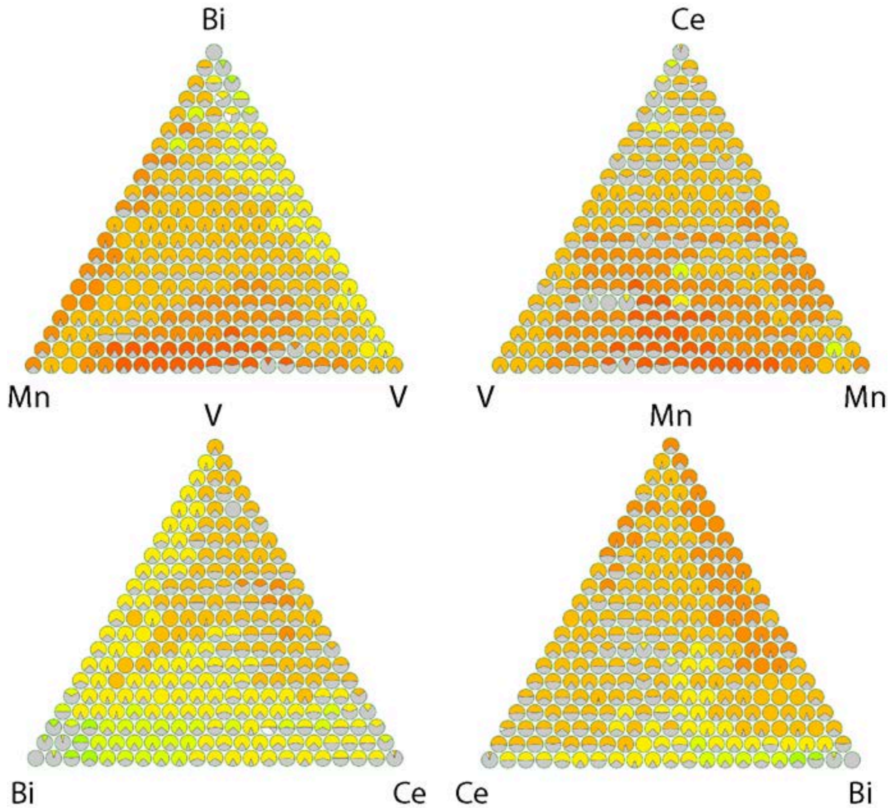

Figure S5. The result of the color screen for the ternary facets of the space, in the representation of Figure 2(c).

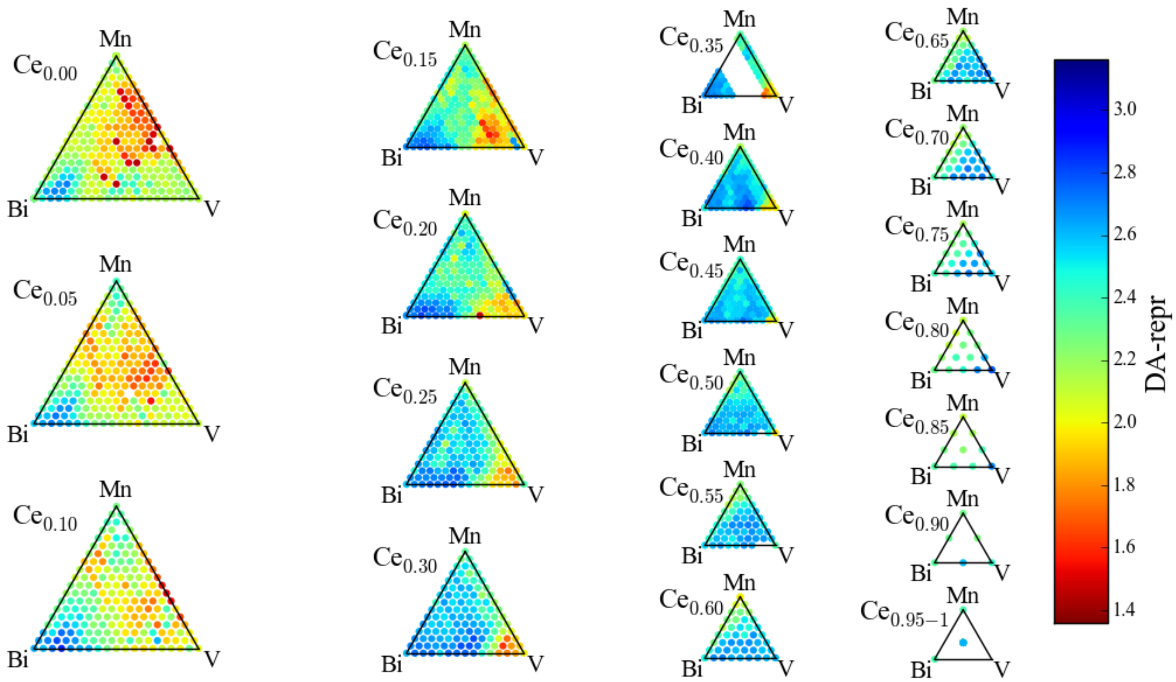

Figure S6. The result of the Tauc analysis for direct allowed bandgap. The scale bar is in electronvolts.

Tauc plot for $Cu_{1.5}Mn_{1.5}O_2$

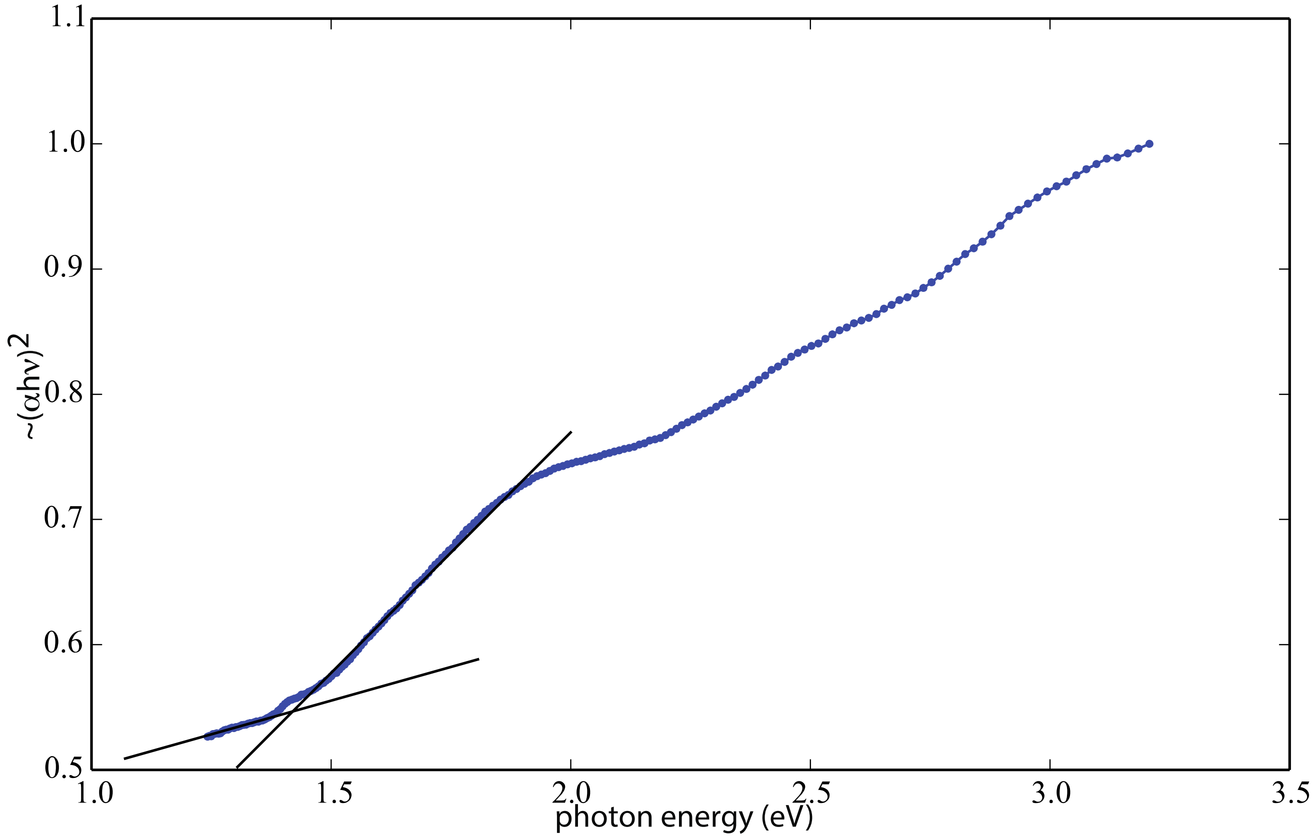

Figure S7. Tauc plot for direct allowed bandgap on one of the Spots with $CuMnO_2$.