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Theoretical efficiency limits of ideal coloured opaque photovoltaics

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Supporting Information

The principle of optimal colour formation for a solar cell

In the following, we show that colours are formed optimally by using sharp reflectance bands that have *R* = 1 within the bands and are placed preferentially in spectral positions where the wavelength-normalized colour-matching functions attain their highest values, while producing the target colour coordinates. As discussed in the paper, two such reflection bands are sufficient to form all possible colours under the finite AM1.5G spectral irradiance. A related proof, not specific to photovoltaic efficiency, but for visual efficiency, has been presented earlier by MacAdam.[1]

In general, the colour of a solar cell is formed optimally when the target *X*, *Y* and *Z* coordinates (of the CIE 1931 colour space) are produced with a minimal number of photons. More precisely, the objective is to reflect primarily wavelengths that maximize colour efficiency, C_{eff}, defined as the ratio between the obtained colour coordinate and the amount of photocurrent lost producing it (equations 2, 3 and 12):

$$C_{eff,Z} = \frac{Z}{J_{ph,loss}} = \frac{hc \int_{360\text{ nm}}^{830\text{ nm}} R(\lambda)[S(\lambda)/\lambda]\bar{z}(\lambda)d\lambda}{q \int_0^{\lambda_g} [R(\lambda) + A_{loss}(\lambda)]IQE(\lambda)S(\lambda)d\lambda} \quad \text{(S1)}$$

where we use the *Z* coordinate as an example, and have taken into account the fact that the colour matching functions are defined for the spectral irradiance $P(\lambda)$ that is related to the photon flux as $P(\lambda) = S(\lambda)hc/\lambda$. Equation S1 is otherwise equivalent to the colour efficiency used by Peharz and Ulm,[2] but is defined here for one colour coordinate, and expressed explicitly in terms of the spectral functions.

Consider next that the spectral reflectance curve $R(\lambda)$ is built up from infinitesimal reflection bands, each having spectral width $\Delta\lambda$. The infinitesimal increment to the *Z* coordinate produced by the band element is

$$\Delta Z = hcR(\lambda)[S(\lambda)/\lambda]\bar{z}(\lambda)\Delta\lambda \quad \text{(S2)}$$

and the corresponding infinitesimal loss in photocurrent density is

$$\Delta J_{ph,loss} = q[R(\lambda) + A_{loss}(\lambda)]IQE(\lambda)S(\lambda)\Delta\lambda \quad \text{(S3)}$$

It follows from equation S1 that the infinitesimal band elements should be placed, the target colour coordinates permitting, in positions that maximize the following incremental ratio

$$\frac{q}{hc}\frac{\Delta Z}{\Delta J_{ph,loss}} = \frac{R(\lambda)}{[R(\lambda) + A_{loss}(\lambda)]IQE(\lambda)}\frac{\bar{z}(\lambda)}{\lambda} \quad \text{(S4)}$$

Notice how the photon flux $S(\lambda)$ cancelled out in this equation. This means that the incident light spectrum has no influence on the order of priority at which the different wavelengths should be reflected to produce the solar colour most efficiently. Instead, wavelengths where the parasitic absorption loss and the internal

quantum efficiency of the cell are lowest, and the value of the colour-matching function is highest, should be prioritized in colour formation. Nevertheless, for an ideal coloured opaque solar cell, characterized by $A_{loss}(\lambda) = 0$ and $IQE(\lambda) = 1$, even the spectral reflectance $R(\lambda)$ cancels out leaving only the wavelength-normalized colour matching function, $\bar{z}(\lambda)/\lambda$, as the measure of the incremental colour efficiency:

$$\frac{q}{hc}\frac{\Delta Z}{\Delta J_{ph,loss}} = \frac{\bar{z}(\lambda)}{\lambda} \qquad \text{(ideal coloured opaque solar cell)} \tag{S5}$$

Naturally, the reflectance within each introduced band element should be always maximal, i.e. $R(\lambda) = 1$, to fully utilize the optimal band position, i.e. to minimize the number of additional reflectance band elements needed to reach the target colour coordinate value, because each additional band element has to be placed at a position that is less optimal than the position of the previous element. Indeed, the target colour coordinate is produced optimally by consecutively adding such infinitesimal unity-reflectance bands to the next-most-optimal unused spectral positions, until the target value of each colour coordinate is reached. Now, because the wavelength-normalized colour matching function $\bar{z}(\lambda)/\lambda$ has only one peak, at 444 nm (Figure S1), this optimization process lead to the formation of a single unity-reflectance band around this peak, with the width of the peak depending on the value of the target colour coordinate and the incident light irradiance spectrum $P(\lambda)$ according to (equation 12 in the paper):

$$Z = \int_{360\ \mathrm{nm}}^{830\ \mathrm{nm}} R(\lambda)P(\lambda)\bar{z}(\lambda)d\lambda = \int_{\lambda_{\mathrm{lo}}}^{\lambda_{\mathrm{hi}}} P(\lambda)\bar{z}(\lambda)d\lambda \tag{S6}$$

where λ_{lo} and λ_{hi} are the lower and higher cut-off limits of the formed reflectance band, and $R(\lambda) = 1$. This reflection band is used primarily for optimal production of the *Z* coordinate, whereas a second band is needed for producing *X* and *Y* coordinates at the longer wavelengths. A third band is not needed, as discussed in the paper, apparently because the $\bar{x}$ and $\bar{y}$ functions overlap so much that their sum has a single peak. In fact, note that the sum of all the colour-matching functions $(\bar{x} + \bar{z} + \bar{y})/\lambda$ has only two peaks (Figures S2), which suggests that two reflection bands are not only sufficient to form all possible colours, but also the optimal way to do so. MacAdam proved this optimality for the colours that have maximum colour purity (saturation), called MacAdam limits, but we believe that this optimality also holds for the colours enclosed by these limits, because they can be produced in an almost identical way, using two distinct reflection bands, as we have done here.

Note that although the illumination spectrum does not affect the order of priority at which different wavelengths should be used in the colour formation, it does affect the width of the reflection bands required to produce the target colour coordinates, and therefore also the associated photocurrent loss, and the solar cell efficiency. For this reason, the same reflectance spectrum that produces a given colour optimally under AM1.5G illumination is not necessarily optimal for producing the same colour under some other (spectrally different, but possibly white) light source spectrum. In fact, it would most likely fail to produce the same colour, due to a phenomenon called metamerism. In other words, although the principle of optimal colour formation is independent of the incident light spectrum, the results of the optimization are different.

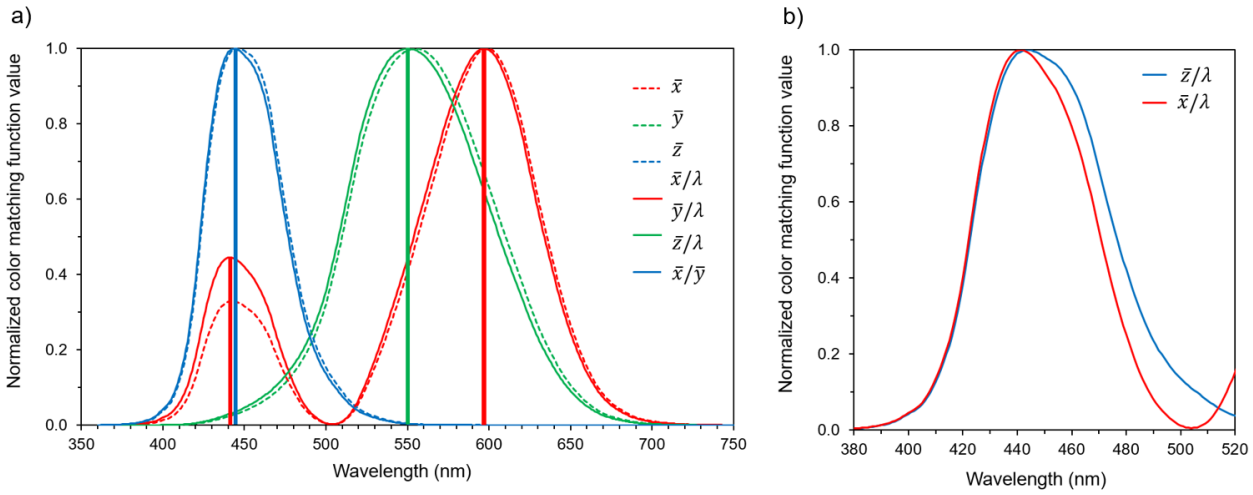

Fig. S1. a) Comparison of the spectral shape of the CIE 1931 2-degree XYZ colour matching functions (dashed lines) and the same functions normalized with the light wavelength (continuous lines). b) Comparison of the shape of the wavelength-normalized $\bar{z}$ and $\bar{x}$ functions. Although figure a) shows that normalizing the colour matching functions by wavelength has a negligible effect on their shape and peak position, the colour optimization was nevertheless carried out based on the wavelength-normalized functions (equation S5).

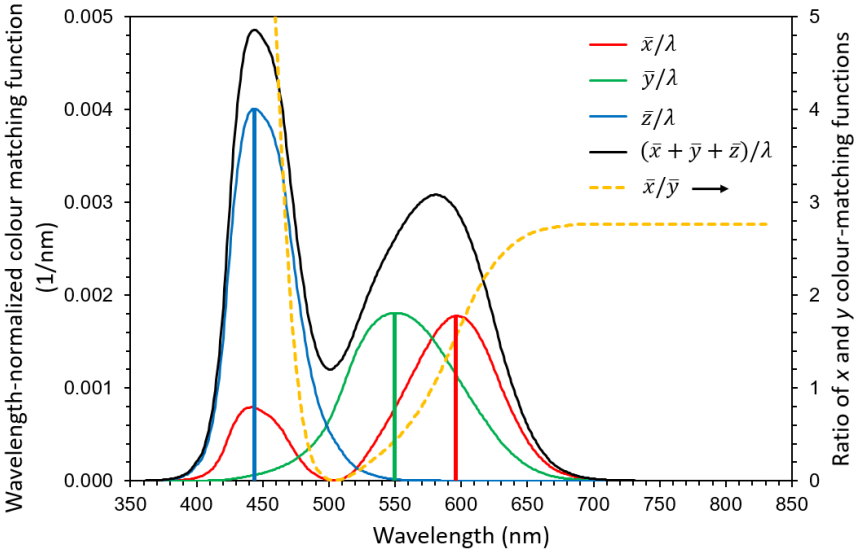

Fig. S2. Absolute values of the wavelength-normalized CIE 1931 2-degree XYZ colour matching functions, their sum, and the ratio between the $\bar{x}$ and $\bar{y}$ functions.

Procedure used for optimizing the colour formation

The iterative colour formation procedure consisted of the following steps:

1. The first reflection band is used to form the *Z* coordinate and is placed at 444 nm where $\bar{z}(\lambda)/\lambda$ achieves its maximal value.
2. This first band is then widened in the direction where $\bar{z}(\lambda)/\lambda$ maintains its highest value until the *Z*-coordinate achieves p = 80 % of its target value.
3. During the widening of the first band, if the value of the *X* or *Y* coordinate exceeds its target value by more than 0.01 %, the first band is narrowed from the side that changes X/Y-ratio towards its correct value.
4. After this, a second reflection band, used for generating *X* and *Y* coordinates, is placed between 505 nm and 670 nm in a position where the ratio $\left(X_t - X_p\right)/\left(Y_t - Y_p\right)$ is correct, where X_t and Y_t are the target colour coordinates, and X_p and Y_p are the colour coordinates produced at this point (after widening the first band). The band is placed between the wavelengths 505 nm and 670 nm because the ratio $\bar{x}/\bar{y}$ achieves values $0.006 < \bar{x}/\bar{y} < 2.77$ there without much altering the Z coordinate. More specifically, the ratio $\bar{x}/\bar{y}$ increases monotonically from 505 nm until it achieves its maximum value at 670 nm, and after this remains constant. On the other hand, when $\bar{x}/\bar{y} > 2.77$ is needed, i.e. when X_t/Y_t is very high (blue to purple colours), the first peak already helps to attain that, because $\bar{x}/\bar{y} > 2.77$ for λ < 467 nm.
5. The second band is widened toward shorter wavelengths if $X_p/Y_p > X_t/Y_t$, and toward longer wavelengths if $X_p/Y_p \leq X_t/Y_t$, until both the *X* and the *Y* coordinates attain more than p = 80 % of their wanted values.
6. During the widening of the second band, if the value of the *Z* coordinate exceeds its target value by more than 0.01 %, the first band is narrowed to maintain the correct *Z* coordinate value, starting from the side where $\bar{z}(\lambda)/\lambda$ has lower value.
7. Steps 2 – 6 are repeated, increasing in each round the target accuracy p, until each of the *X*, and *Y* and *Z* coordinates attain 99.99 % < p < 100.01 % of their target values. Nine rounds of the steps 2 – 6 were enough to reach the desired accuracy. The target accuracy was p = 80 %, 90 %, and 95 % for the first three rounds and thereafter 99.99 % for six rounds.

Numerical accuracy of the calculations

All calculations were performed using the following numerical resolutions and accuracy:

- The original resolution of the used spectral data was 1 nm for the AM1.5G spectrum (0.5 nm below 400 nm, and 5 nm above 1700 nm) and the colour matching functions, which was interpolated into 0.02 nm steps for the spectral calculations.
- The reflection band edge positions were optimized using 0.2 nm wavelength increments.
- Band-gap was optimized using 0.5 meV steps.
- Maximum power-point voltage was optimized using 1 μV or better accuracy.

These numerical resolutions were chosen to ensure accuracy of the calculated theoretical efficiency limits within four significant digits.

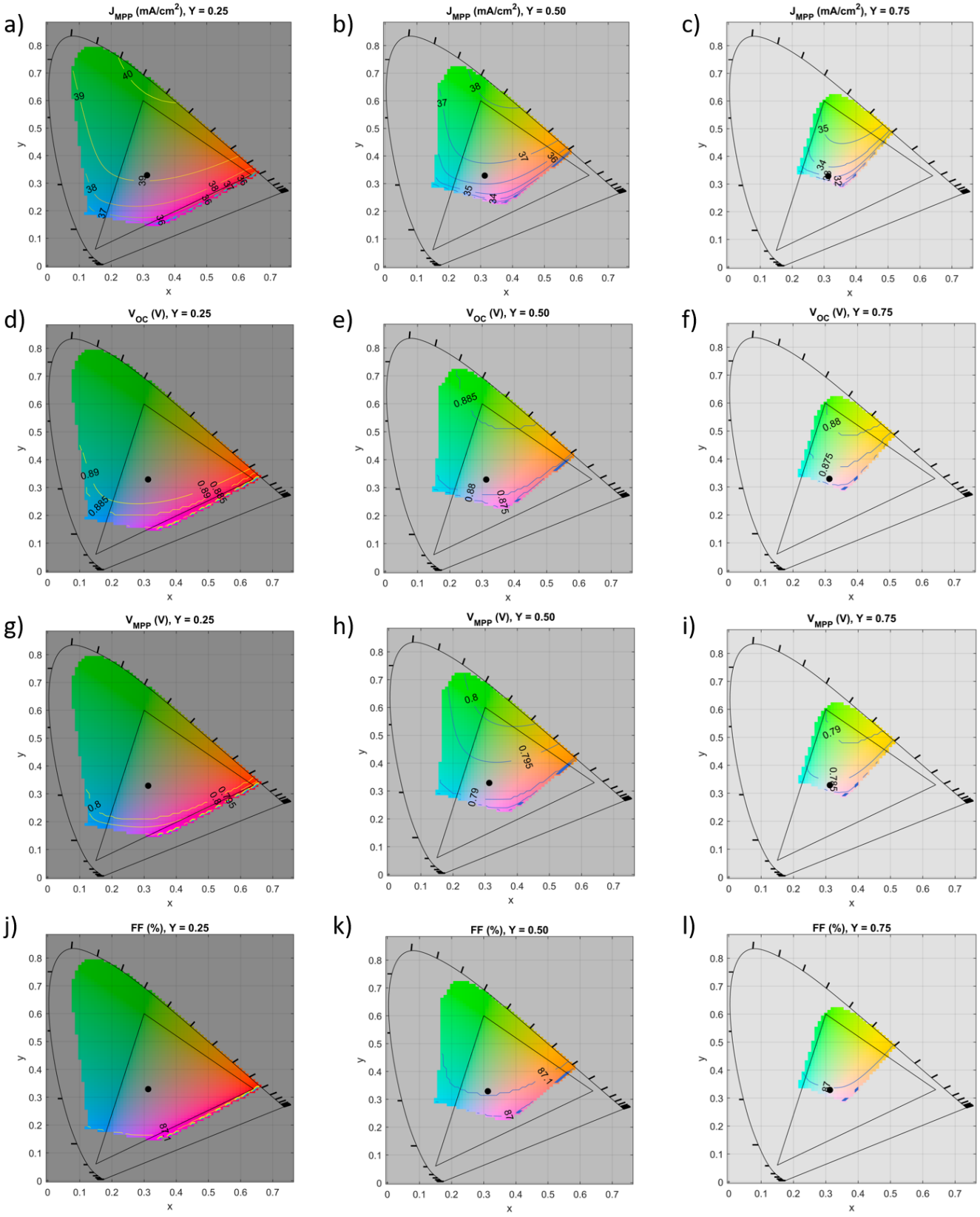

Fig. S4. Collection of figures corresponding to those in Fig. 3 in the paper, showing maximum power-point current density J_{MPP} (a-c), open circuit voltage V_{OC} (d-f), maximum power point voltage V_{MPP} (g-i), and fill factor *FF* (j-l).

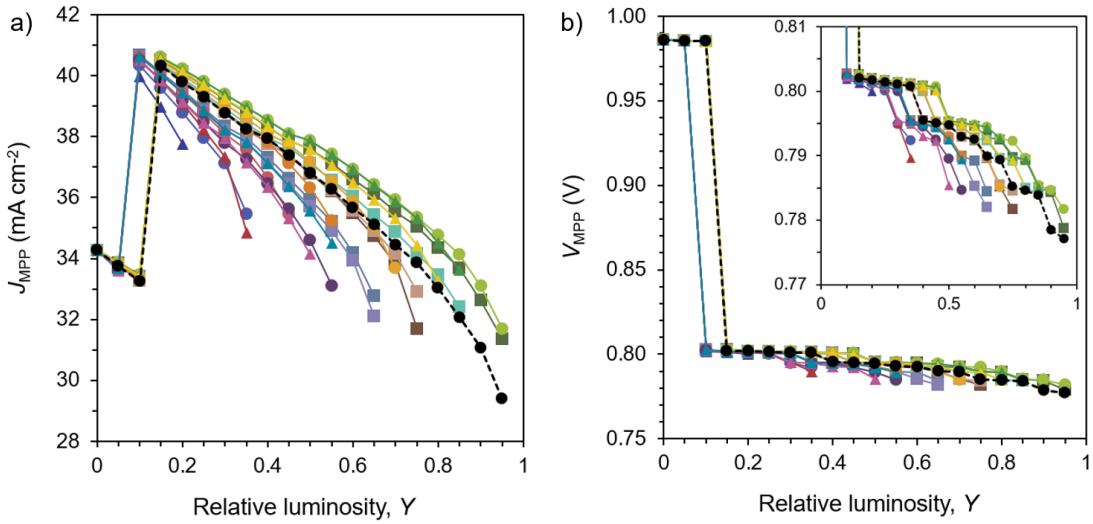

Fig. S3. Figures corresponding to those in Fig. 4 in the paper, showing a) maximum power-point current density J_{MPP} and b) maximum power point voltage V_{MPP}.

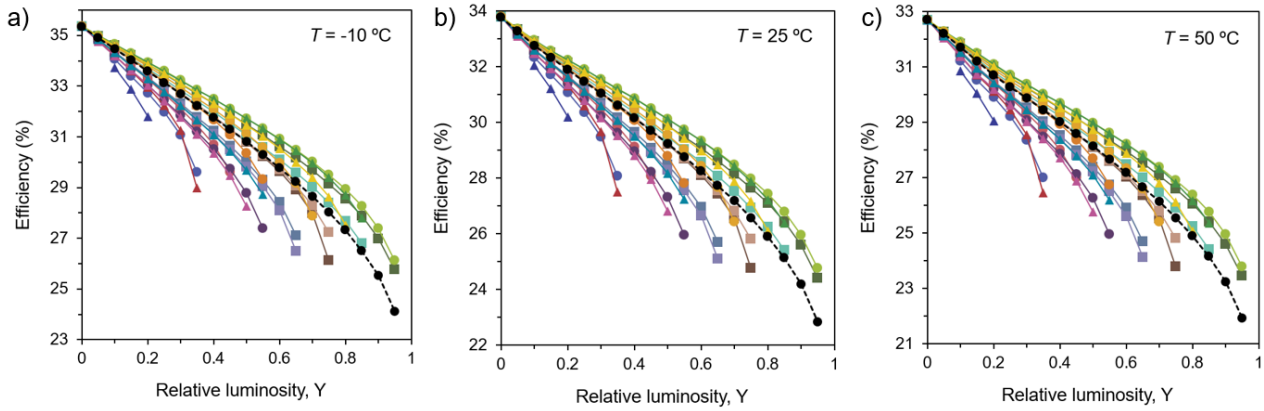

Fig. S4. Effect of temperature on the theoretical efficiency limits of the selected colours used in Fig. 4 in the paper. It can be seen that the temperature does not affect the colour dependence of the efficiency limits: the figures a) – c) are almost identical, except that the data are shifted along the efficiency axis due to different temperature (marked in the figures). This result is expected temperature affects only the recombination current (eqs. 5 – 7 in the paper) and not the photocurrent (eqs. 2 and 4 in the paper) that almost exclusively determines the colour dependency of the results.

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2. Peharz G, Ulm A. Quantifying the influence of colors on the performance of c-Si photovoltaic devices. *Renew Energy*. 2018;129:299-308. doi:10.1016/j.renene.2018.05.068