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Supplementary Information for "On efficiency of perovskite solar cells with a back reflector: Effect of a hole transport material"

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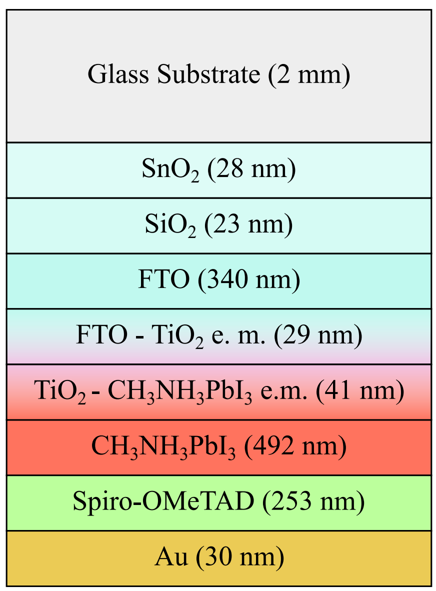

Figure 1: Schematic planar heterojunction configuration studied by Ball et al.[1], where the symbol "e.m." is the effective media.

To validate our approach, we use the experimental data from Ref.[1], provided for the p-i-n planar heterojunction configuration for a perovskite–based solar cell, shown in Fig.1. The device was illuminated with a solar simulator, which has the spectrum shown in Fig. S6 of Ref.[2], equivalent to 1.047 suns.

We recall that in Ref.[1] the optical properties have been analysed within an optical model based on the transfer-matrix formalism, using experimentally determined complex refractive index data. Our analysis of optical properties are done by means of the Monte-Carlo ray tracing simulations complemented by the transfer-matrix method (OTSun python package [3]). We use for each layer of the device the complex refractive index spectra, provided by Refs.[1],[2]. All calculations are done for a specular reflection case. In all figures, presented below, our results are indicated by the red color, while those from Ref.[1] are indicated by the green color.

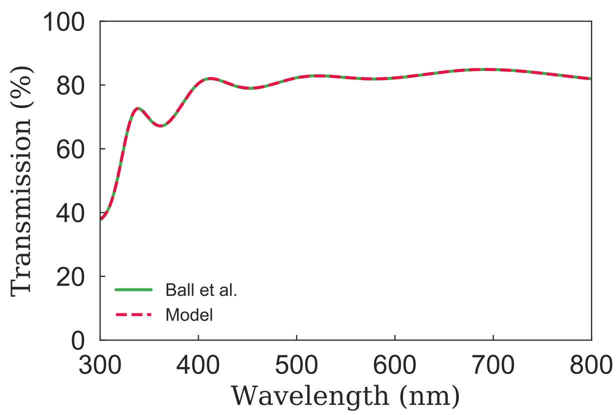

Figure 2: The comparison of the FTO-coated soda-lime glass substrate transmission spectrum obtained by Ball et al. [1] and by means of our TMM model implementation.

In order to determine the wavelength power transmission of the FTO-coated soda-lime glass substrate used in Ref.[1], we compare our TMM simulations with that, provided by Ref. [2] (see Fig.S1a, Ref.[2]). Evidently, the results are equivalent (see Fig.2), since the both TMM models are based on the Python library developed by Steve Byrnes [4]. The same agreement is obtained (see Fig.3) between our result for the reflectance and that, presented in Fig. 6 of Ref.[1]. Next important characteristic is the light-harvesting efficiency (LHE). It is obtained by means of the TMM in Ref.[1], while our results are obtained with the aid of the ray tracing simulations complemented by the TMM. The comparison between our results and those, presented in Fig.4a of Ref.[1], demonstrates a good agreement as well (see Fig.4). Note, however, that our model gives a slightly lower LHE. In our case the perovskite and Spiro-OMeTAD are considered as incoherent media.

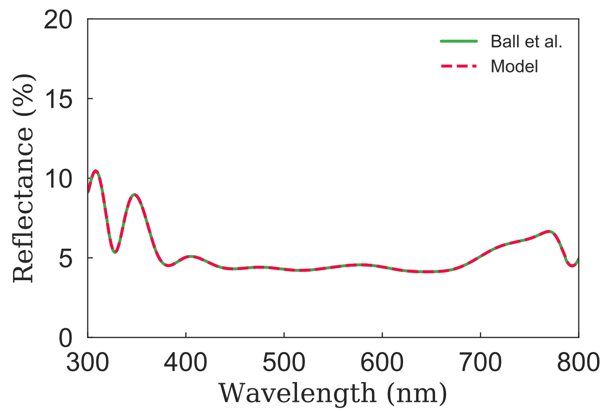

Figure 3: The comparison of the calculated reflectance spectra obtained by Ball et al.[1],[2] and by means of our TMM model implementation.

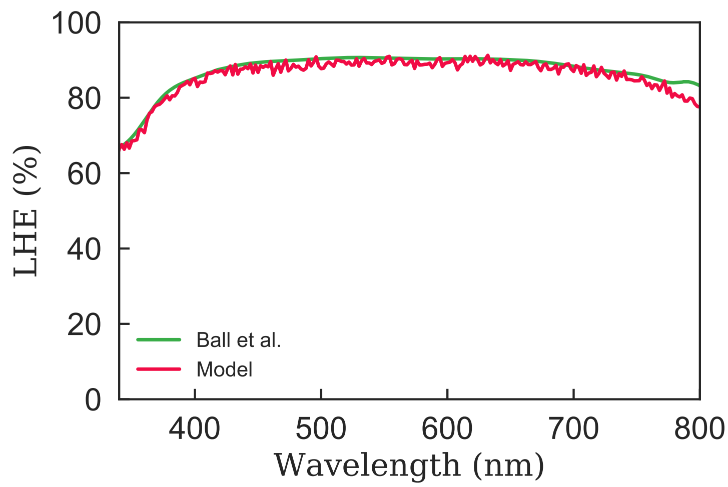

Figure 4: The comparison of the light-harvesting efficiency, obtained in Ref.[1], and our LHE, obtained by means of the ray tracing+TMM approach (the OTSun package) [3].)

To demonstrate the relevance of our model J(V) characteristic to experimental observations, we use the analogy of the PSC to a current generator in parallel with a diode. In addition, it is necessary to account for the parasitic resistance of the contacts and feeding conductors, R_s; the leakage resistance R_{sh} related to the local short circuit of ETM/HTM layers. Thus, we analyse the equivalent circuit, shown in Fig.5. The intrinsic PSC current J_d+J_{sc} is evaluated by means of the numerical solution of the transport equations

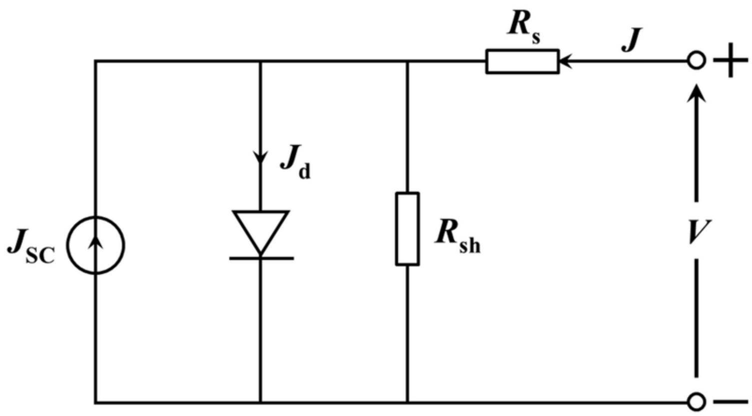

Figure 5: The circuit layout: i)R_s is a parasitic resistance of contacts and feeding conductors; ii)R_{sh} is associated with a leakage resistance related to the local short circuiting of ETM/HTM layers; iii)J_d is a dark current; iv)J_{sc} is a photogenerated current. The intrinsic PSC current is J_d+J_{sc}.

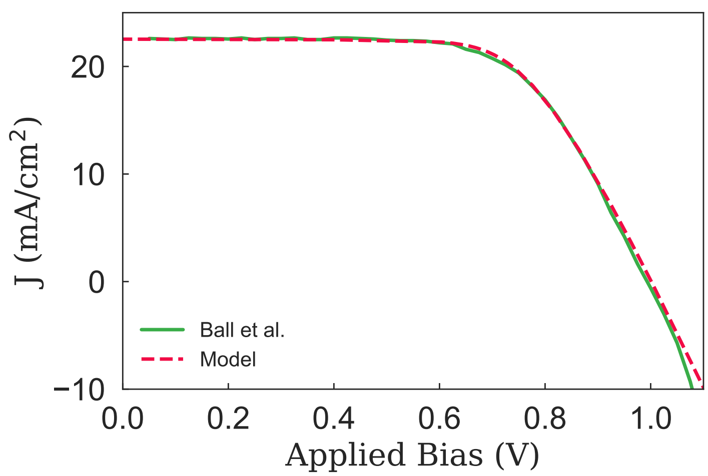

Figure 6: Measured and simulated J-V characteristics of the device used for validation.

(6-13), where we use the results of the optical calculations of the photogeneration rate $G(z)$ (Eq.5) as the input. The electrical parameters have been taken from Table 1 of our paper. To reproduce the open circuit voltage value of the PSC [1], we use the diffusion length $\ell_D = 2\mu$m for the perovskite. Additionally, the best agreement between our and measured results for the short curcuit current is obtained if we use the diffusion length

	PCE%	J_{sc}, mA/cm^2	V_{oc}, V	FF	J_{tot},mA/cm^2
Simulated	14.19	22.56	1.00	0.66	24.80
Experiment	13.80	22.60	1.00	0.64	

Table 1: Simulated and measured main characteristics of the PSC [1].

$\ell_D = 0.04\mu$m for TiO_2. The best fit of the simulated and measured J–V characteristics is obtained with R_s=8 Ohm·cm^2 and R_{sh}=10 MOhm·cm^2. The comparison of the result for the J–V characterisitics with that from Ref.[1] is displayed on Fig.6. Finally, Table 1 demonstrates the remarkable agreement between the model calculations and the experimental data. Thus, the comparison between our results for the optical and the electrical characteristics and those, provided by Ref.[1], demonstrates the vitality and the validity of our model.

References

[1] J.M. Ball, S.D. Stranks, M.T. Hörantner, S. Hüttner, W. Zhang, E.J.W. Crossland, I. Ramirez, M. Riede, M.B. Johnston, R.H. Friend, H.J. Snaith, *Optical properties and limiting photocurrent ofthin-film perovskite solar cells*, Energy Environ. Sci.**8** (2015) 602-609. doi:10.1039/C4EE03224A

[2] J.M. Ball et al., Energy Environ. Sci.**8** (2015) 602-609; Electronic Supplementary Information (ESI): Detailed description of methods, supplementary discussion sections S1-S3, Figures S1-S11, transfer-matrix code, and modelling data.

[3] G. Cardona, R. Pujol-Nadal, *OTSun, a python package for the optical analysis of solar-thermal collectors and photovoltaic cells with arbitrary geometry*, PLOS ONE **15** (2020) e0240735. doi:10.1371/journal.pone.0240735.

[4] Steven Byrnes, tmm 0.1.7: ”Python Package Index”, https://github.com/sbyrnes321/tmm.