Area 5: Perovskite Solar Cells.

A SPATIALLY SMOOTHED DEVICE MODEL
FOR MESO-STRUCTURED PEROVSKITE SOLAR CELLS

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Meso-structured perovskite solar cells (meso-PSCs), utilizing a mesoporous absorber layer consisting of mesoporous perovskite material and mesoporous titanium oxide (TiO₂), see Fig.1b, are still delivering the highest solar cell efficiencies for perovskite solar cells up to date [1]. The performance of meso-PSCs critically depends on the nanoscale morphology formed inside this mesoporous layer. This however is not accounted in most device simulation programs, as they are based on an effective medium approximation for the mesoporous absorber layer, which ignores the details of its underlying morphology. The mesoporous absorber layer is treated as a two-phase model (mesoporous perovskite and mesoporous TiO₂) that describes intrinsic solar cell physics such as free charge carrier generation, carrier transport and recombination under various illumination intensities (0.3 sun, 0.5 sun and 1 sun) and five interfaces. A subsequent recombination loss analysis (under maximum power and open circuit condition) will be investigated to identify the dominant recombination loss occurring under open-circuit condition. This work derives a spatially smoothed device model for meso-PSCs, based on volume-averaging theory of the two-phase model as developed by Whitaker [2] for the transport of chemical species through a porous media. The two essential morphological parameters of the mesoporous layer (that cannot be found in existing effective medium models) are: (1) the porosity $\phi$ and (2) the effective interfacial area $A_v$ (defined as the surface area per unit volume).

![Graph](image)

Figure 1: (a) Simulated (lines) and measured (symbols) current-voltage curves for meso-PSCs under an AM 1.5 solar spectrum at 1 sun (▲), 0.5 sun (■) and 0.3 sun (▼) illumination intensity. (b) Schematic of a meso-PSC, considering six layers and five interfaces. (c) Recombination loss analysis under open-circuit condition. (d) Simulated current-voltage curves for structures that corresponds to $A_v$ values of $[0.25, 1.4, 8, 16] \times 10^{-9}$ m$^{-1}$. The arrow indicates an increasing value of $A_v$. The symbol (▲) indicates the measured current-voltage curve at 1 sun.

At the conference, differently processed meso-PSCs from various collaboration partners will be analyzed and compared. To give an example here, we apply device modelling using spatial smoothing on our own experimental data presented previously, introducing a loss analysis for meso-PSCs [3]: First the simulation is calibrated towards intensity dependent current-voltage curves taken at various illumination intensities (Fig.1a). A corresponding data fitting will allow to fix the morphology parameters (porosity $\phi$ and interfacial area $A_v$) within the experimentally given range. An increase in the interfacial area $A_v$ corresponds to an increase of interface recombination and thus to a decrease in fill-factor (Fig. 1d). A subsequent recombination loss analysis (under maximum-power and open-circuit conditions) can identify the dominant loss channels of the investigated meso-PSCs (Fig. 1c).

For the meso-PSCs analyzed thus far, the interfacial recombination within the mesoporous absorber layer dominates over all other recombination loss channels. This corresponds well with our earlier work [3] and also with experimental evidence [4], indicating an interfacial potential barrier formed between the perovskite and the TiO₂. As an example, the recombination losses under open-circuit conditions are shown in Fig. 2(b): 37% recombination loss occurs at the perovskite/TiO₂ interface in the mesoporous layer; 35% at the perovskite capping layer; 16% at the perovskite capping layer/hole-transporting layer interface; 12% at the perovskite material within the mesoporous layer. Thus, an appropriate surface treatment to minimize the mesoporous TiO₂/perovskite interface recombination is crucial for the device performance.