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Light management for absorption enhancement in PbS quantum dot solar cells

Stefan Wil Tabernig[1], Zhi Li Teh[2], Andrea Cordaro[1], Rob Patterson[2], Gavin Conibeer[2], Shujuan Huang[2] and Albert Polman[1]

[1]Center for Nanophotonics, AMOLF, Science Park 104, 1098 XG Amsterdam, the Netherlands
[2]Australian Centre for Advanced Photovoltaics (ACAP), School of Photovoltaic and Renewable and Engineering University of New South Wales, Sydney 2052, Australia
E-mail: s.tabernig@amolf.nl

PbS quantum dot solar cells (QDSCs) belong to the group of promising emerging photovoltaic technologies. The reason for their popularity stems from the fact that their bandgap can be tuned across the visible spectrum and the ease of fabrication which is based on a solution-deposition process. Furthermore, PbS QDSCs require only a very thin absorption layer of usually sub-micron thickness. This means that large-scale flexible PbS QDSC-modules have the potential to be inexpensive, as a small amount of raw material is required for their fabrication. To further reduce cost and flexibility it would be beneficial to further thin down the PbS layer. However, this leads to a loss of absorption in the active layer, especially for wavelengths towards the red/infrared.

To address this issue, we propose an improved design for the interface between the absorbing PbS QD layer and the ZnO layer (Figure 1). By patterning the ZnO layer prior to the QD deposition, we simultaneously employ two mechanisms. Firstly, the enhancement of the interface-area due to the patterning can potentially improve the charge carrier collection efficiency[1,2]. Secondly, the dimensions of the pattern are chosen such that PbS QD pillars - surrounded by ZnO - are formed. The refractive index contrast between the PbS QDs and ZnO allows for enhanced coupling of light into the QD pillars. Quantitatively, this is expressed as an optical cross section being larger than the geometrical cross section of the QD pillar. By tuning this system such that the optical cross section is large across the wavelength range between the first exciton peak and the onset of the bulk absorption, we address inefficient absorption in that specific range, while keeping the required absorber volume minimal.

As can be seen in Figure 2, the absorption profile of the patterned PbS QD layer shows a steep onset, similar to direct bandgap semiconductors, and no dip in absorption for wavelengths slightly below the first exciton peak. Moreover, the absorption is enhanced over the full range. This is achieved via two mechanisms. First, the height of the QD pillar allows for higher-order Fabry-Pérot resonances to occur. The large optical cross section leads to concentration of the electric field inside the QD pillar, at the expense of the volume filled up by ZnO. Figure 3 shows this for a wavelength of 800 nm. The dip around 800 nm which can be seen for the absorption spectrum of the flat QD layer in Figure 2 is cancelled out in the patterned case, due to light concentration inside the QD-pillar via shifting of the Fabry-Pérot resonance towards this wavelength.

Additionally, this design profits from the fact that the periodic nature of the pillars allows for coupling into quasi-guided modes at specific wavelengths. This leads to sharp peaks in the absorption spectrum at 750, 900 and 950 nm (see Figure 2). Evidence for the dependence on the periodicity of these quasi-guided modes can be found by sweeping the QD pillar pitch, as shown in Figure 4. Three sharp resonances intersect the 500 nm pitch line at the wavelengths mentioned above. The placement of these modes was chosen such that the two longer-wavelength modes enhance absorption at the red-tail of the first exciton peak while the shortest wavelength mode is placed such that it cancels out a dip that occurs around 750 nm.

These simulations will be the basis for the fabrication of such a PbS solar cell, which will be done via substrate-conformal soft-imprint lithography. In combination with reactive ion etching, this technique allows for nano-patterning of the ZnO layer. Subsequent to the patterning, the PbS QD solution will be spin-coated onto the pattern and the cell is finalised with the evaporation of a Au back contact. EQE measurements will allow for a direct comparison of experimental and simulated absorption and experimental JV-characteristics will unveil how beneficial such a design can be for the overall performance of QD solar cells.

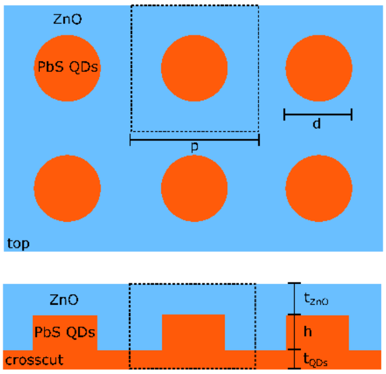

Figure 1: Horizontal cross-cut through the ZnO and PbS QD layers (top). Vertical cross-cut through the same layers (bottom).

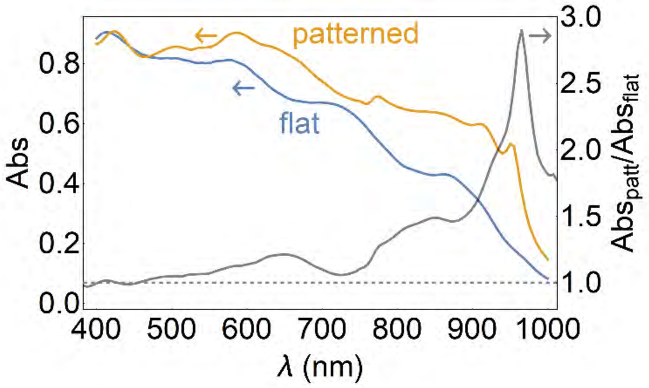

Figure 2: Calculated absorption of a flat (blue) and patterned (yellow) PbS QD solar cell for the same QD volume, corresponding to a thickness of 180 nm for the flat cell. The relative absorption enhancement is shown in grey.

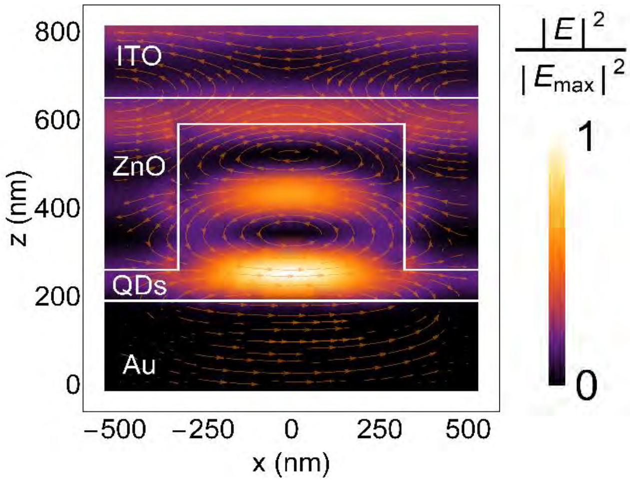

Figure 3: Electric field intensity distribution across the QD solar cell. The incident electric field is polarized along the x-axis and propagating downwards along z. The in-plane electric field components are indicated with field lines.

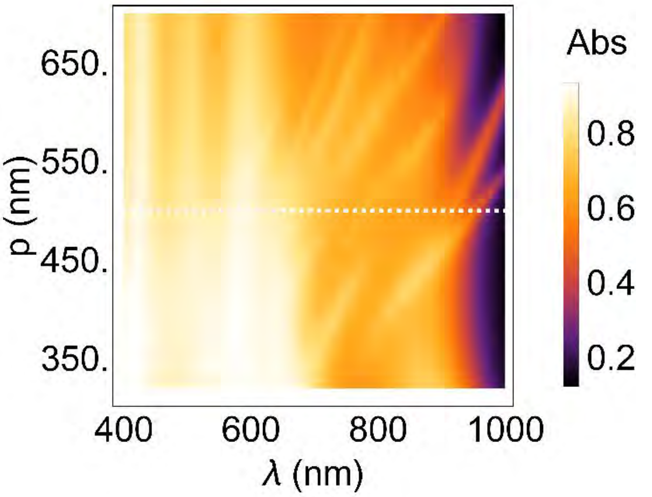

Figure 4: Absorption as a function of wavelength for different QD-pillar pitches. The white dashed line indicates the pitch chosen for the final design (500 nm).

References

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2. Kawawaki, T. *et al.*, 2015, Efficiency Enhancement of PbS Quantum Dot/ZnO Nanowire Bulk-Heterojunction Solar Cells by Plasmonic Silver Nanocubes, *ACS Nano*, 9, p4165-4172