Benefits of photonic structuring on perovskite solar cells using opal-like layers

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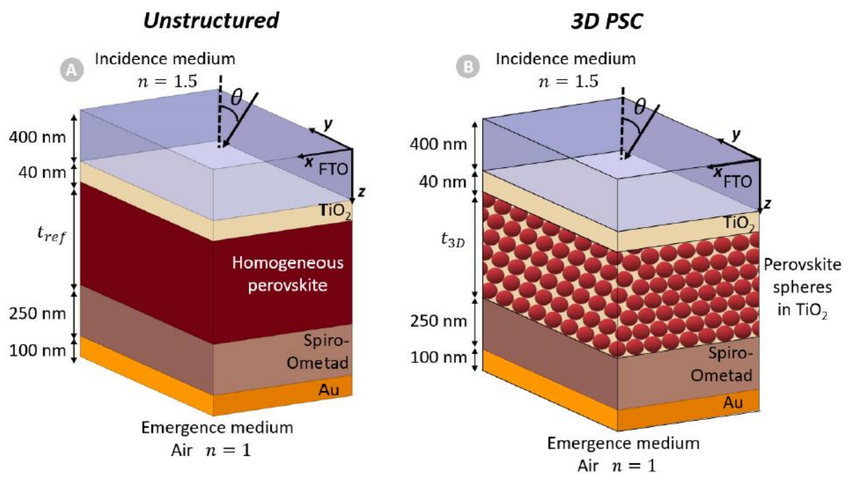
Abstract

Perovskite solar cells (PSC) have been under the spotlight of the photovoltaics community since the past decade due notably to high instrinsic absorption of pervoskite. However, little is known on the impact of structuring the active material using photonic crystal layers. We present here numerical simulations showing the effect of photonic crystal structuring on the integrated quantum efficiency of perovskite solar cells. The photo-active layer is structured using opal-like perovskite layers (monolayers, bilayers or trilayers) made of perovskite (full or truncated) spheres, including hybrid uniform/structured layers, embedded in a TiO_2 matrix. Fano resonances are exploited in order to enhance the absorption, especially near the electronic bandgap of perovskite material. The excitation of quasi-guided modes inside the absorbing spheres increases the integrated quantum efficiency and the photonic enhancement factor. A genetic algorithm approach allows us to determine the optimum structure among more than $1.4\ 10^9$ potential combinations. These numerical results of the benefits of photonic structuring on perovskite solar cells are also compared to experimental studies on selected configurations of perovskite solar cells.

Photonic structures and materials



Role of the different layers

- FTO: transparent conducting electrode
- TiO_2 : hole blocking layer
- Perovskite $CH_3NH_3PbI_3$ layer: photo-active layer (unstructured vs 3D structuration)
- Spiro-Ometad: hole transporting layer
- Au: counter-electrode and back reflector

Goals

- ✓ ***Compare the effect of 3D structuring vs unstructured photo-active perovskite layer on the integrated quantum efficiency (iQE η)***
- ✓ ***Optimize absorption using a Genetic Algorithm (GA)***
- ✓ ***Confirm the numerical prediction experimentally***

Numerical methods and figures of merit

- Numerical simulations are performed using the Rigorous Coupled Wave Analysis (RCWA) method [1]
- The global absorptance $A_g(\lambda)$ is deduced from the energy conservation law: $A_g(\lambda) = 1 - R(\lambda) - T(\lambda)$

- Two figures of merit (FOMs):

  - ✓ ***Integrated quantum efficiency η*** : represents the percentage of incident photons that are absorbed in the whole structure

$$\eta = \frac{\phi_A}{\phi_{inc}} = \frac{\int_{\lambda_{min}}^{\lambda_{max}} \frac{\lambda}{hc} S(\lambda) A_g(\lambda) d\lambda}{\int_{\lambda_{min}}^{\lambda_{max}} \frac{\lambda}{hc} A_g(\lambda) d\lambda}$$

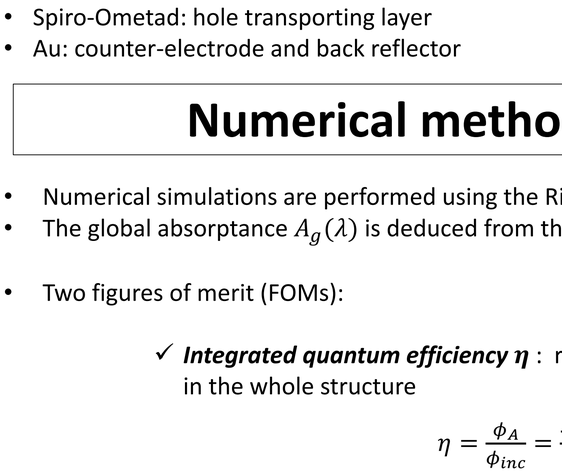
where ϕ_A (ϕ_{inc}) is the spectrally integrated absorbed (incident) photon flux, $S(\lambda)$ is the normalized solar spectrum AM1.5G, $\lambda_{min} = 310\ nm$ and $\lambda_{max} = 800\ nm$ corresponding respectively to the lower bound of the solar spectrum and to the perovskite band gap.

  - ✓ ***Photonic gain*** G_{phot}: evaluates the enhancement of the generation of photo-electrons due to the photonic structuring in comparison with an equivalent unstructured photonic slab structure

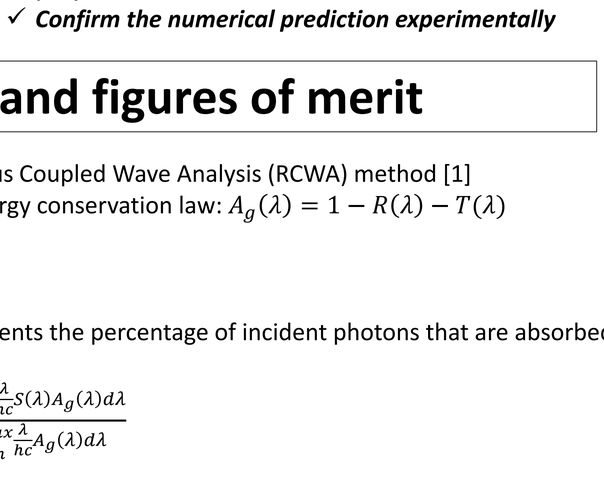
$$G_{phot} = \frac{\phi_{3D} - \phi_{\mathrm{hom}}}{\phi_{\mathrm{hom}}} \times 100$$

Entire perovskite spheres in an hexagonal array

Spectra for monolayers of spheres with different radii



FOMs for 1,2,3 layers



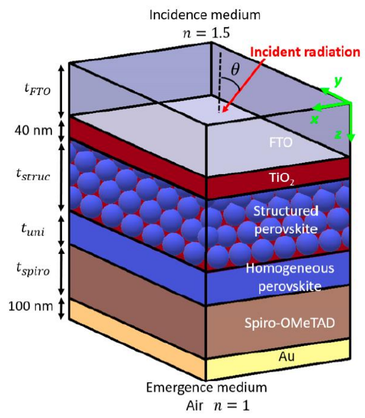
✖ = optimum G_{phot}

Maxima of photonic enhancement factor with corresponding radii and iQE, for 1,2 and 3 layers

N	$G_{phot}^{Max}[\%]$	$R_{Max}[nm]$	$\eta[\%]$
1	6.4	175	88.6
2	4.3	50	79.3
3	3.6	200	96.7

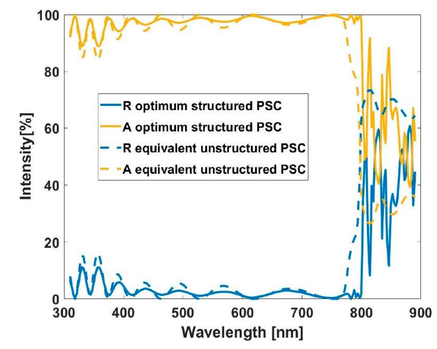
Benefits of photonically structuring the photo-active perovskite layer [1]

Optimization using a Genetic Algorithm



- Slightly modified structure:
  - ✓ Supplementary homogeneous perovskite layer between the structured perovskite layer and the Spiro Ometad layer
  - ✓ Perovskite spheres are allowed to be non-entire, i.e truncated
- GA optimization among $1.4\ 10^9$ potential combinations [2,3,4]
- Parameters to optimize [allowed range]:
  - ✓ t_{FTO} [50-800 nm]
  - ✓ t_{uni} [0-100 nm]
  - ✓ R (radius of spheres) [50-1100 nm]
  - ✓ t_{struc} [50-2200 nm]
  - ✓ t_{Spiro} [50-800 nm]

Results



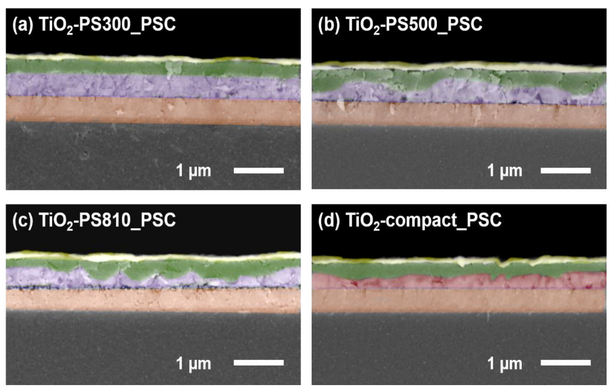
Optimum parameters provided by the GA optimization process.

Parameter Name	Optimum Value
Thickness of the transparent conducting electrode fluorine-doped tin oxide *FTO* layer t_{FTO}	710 nm
Thickness of the uniform perovskite layer t_{uni}	80 nm
Radius of the perovskite spheres R	300 nm
Thickness of the structured perovskite layer t_{struc}	2080 nm
Thickness of the hole transporting spiro–OMeTAD layer t_{spiro}	240 nm

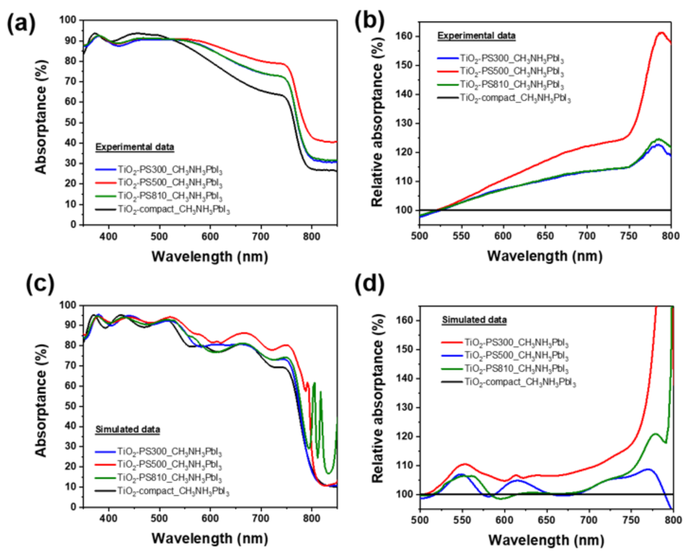
$\eta_{opt} = 98.1\%$

Enhanced iQE using GA [2]

Experimental confirmation



- Photonically-structured TiO_2 is considered as photoanode layer for perovskite $CH_3NH_3PbI_3$ solar cells [5]
- Three radius are considered: $R{\sim}110\ nm$; $R{\sim}200\ nm$; $R{\sim}305\ nm$ (referred to as PS300, PS500 and PS810 here) and an homogeneous/compact layer for control



- Optimum for $R{\sim}200\ nm$ is found on the absorptance spectra, close to the numerical optimum [1]
- Important relative absorptance enhancement close to the electronic bandgap as expected
- Due to the occurrence of electronic-related counter-effects not taken into account into numerical simualtions, the $R{\sim}110\ nm$ shows an higher power conversion efficiency (${\sim}10\%$) than the $R{\sim}200\ nm$ [5].

References

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