LEAP-RE STAKEHOLDER FORUM THEMATIC SESSIONS

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LEAP-RE

Long-Term Joint EU-AU Research
and Innovation Partnership on Renewable Energy

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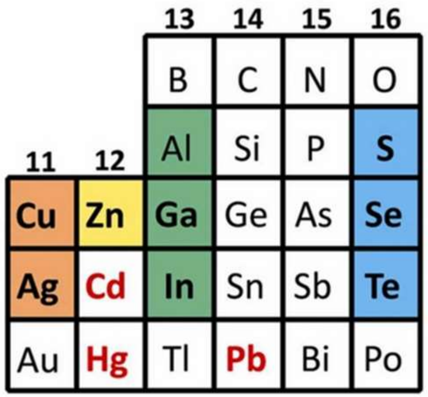
Compositional engineering of highly emissive and widely tunable I-III-VI_2 quantum dots (QDs) for photovoltaic applications

I-III-VI$_2$: synthesis and optical properties

Nomenclature



		13	14	15	16
		B	C	N	O
11	12	Al	Si	P	S
Cu	Zn	Ga	Ge	As	Se
Ag	Cd	In	Sn	Sb	Te
Au	Hg	Tl	Pb	Bi	Po

Binary QDs

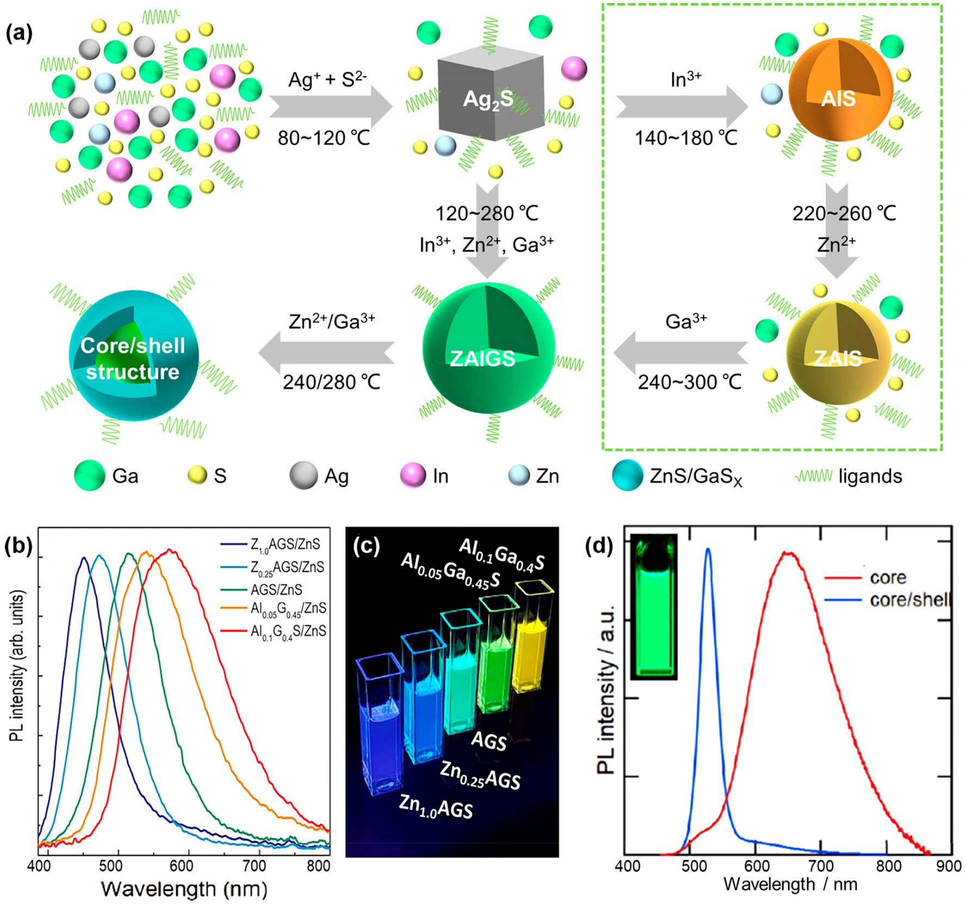
- II-VI (CdS, CdSe, CdTe, ZnS)
- III-V (InP, GaP, InAs)
- IV-VI (PbS, PbSe, SnS)

Ternary QDs

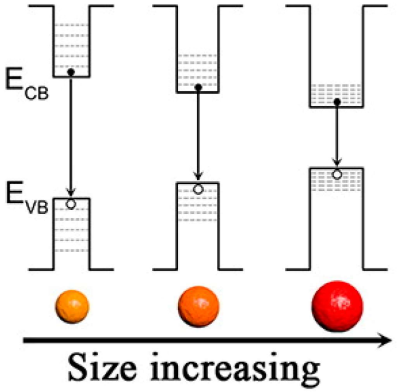
- **I-III-VI** ($CuInS_2$, $AgInS_2$, $CuGaSe_2$)

Nano Lett. 2023, 23, 7, 2443–2453.

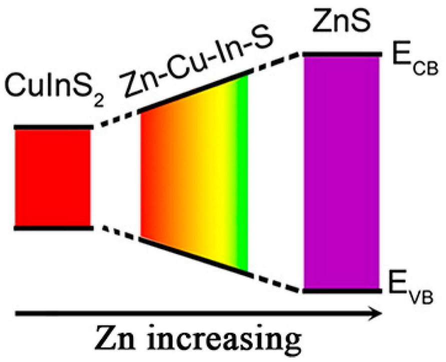
Synthesis



Size Tuning

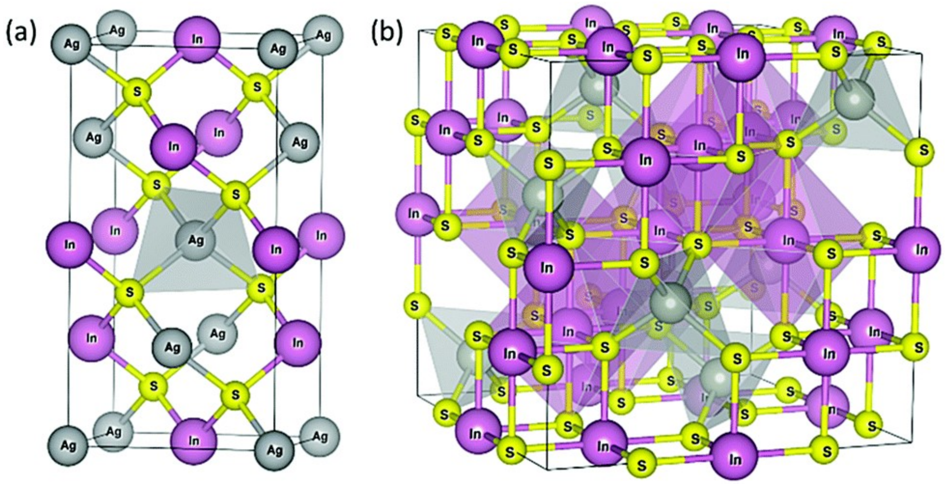


Composition Tuning



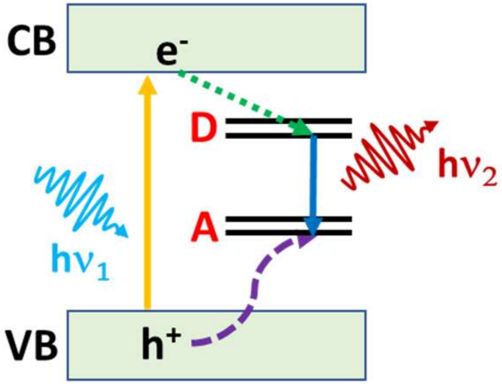
I-III-VI_2 : synthesis and optical properties

High tolerance to off-stoichiometry. Ex: $AgInS_2$ QDs



lattice rich in crystallographic defects
(interstitial atoms, vacancies and antisite defects).

Ag vacancies (V_{Cu}), sulfur vacancies (V_S),
Ag interstitial atoms (Ag_{nt}) and sulfur interstitial atoms (S_{int})



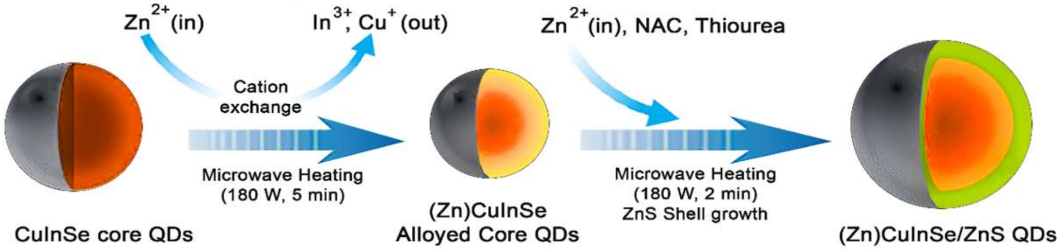
V_s and Ag_{int} as donors

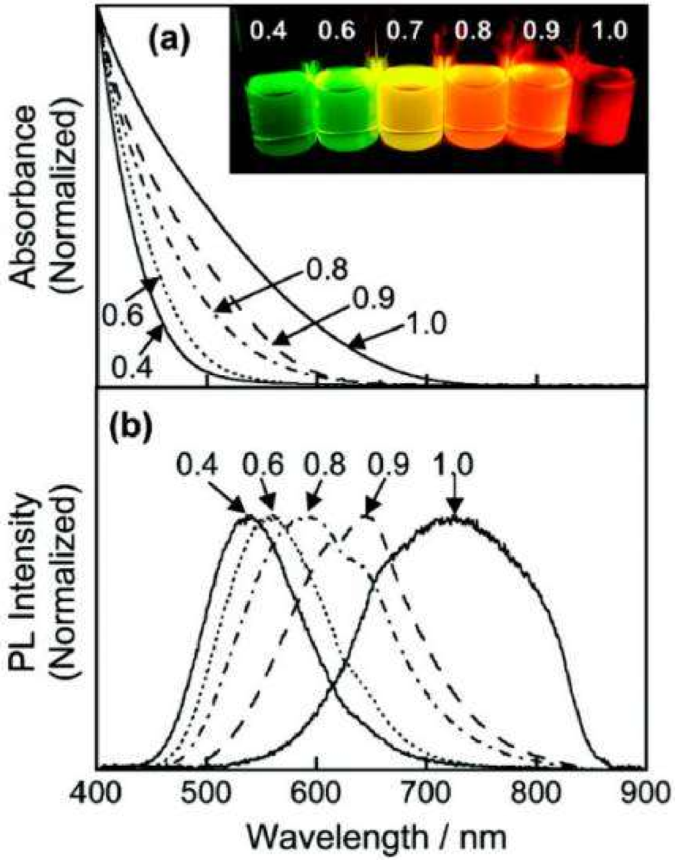
V_{ag} and S_{int} as acceptors

dominated by radiative recombination linked to donor-acceptor (D-A) defects but also by surface-related defects due to the high surface-to-volume ratio of these nanocrystals

I-III-VI$_2$: synthesis and optical properties

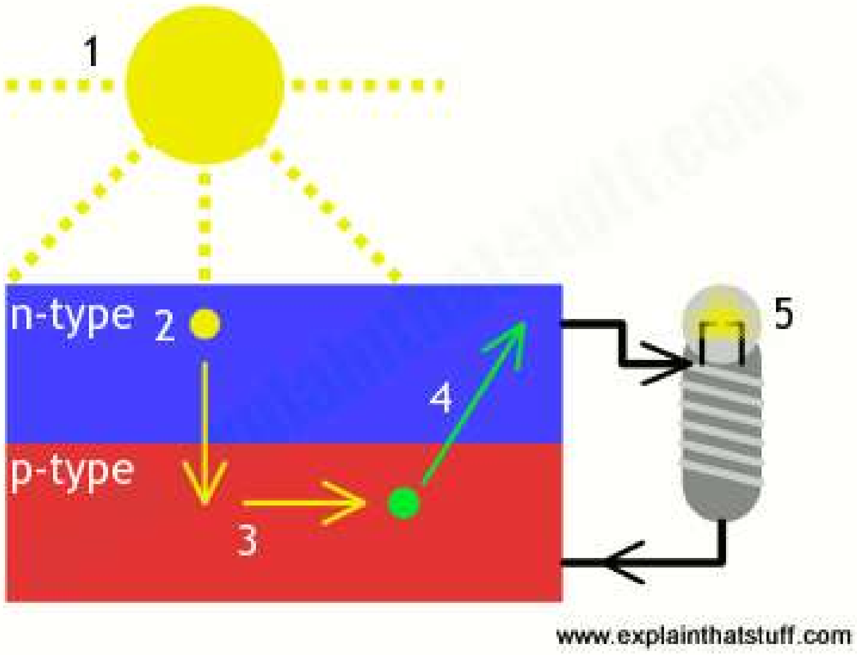
Alloying during shelling





Absorption spectra (a) and PL spectra (b) of AIS/ZnS QDs obtained from the decomposition of precursor $(AgIn)_xZn_{2(1-x)}(S_2CN(C_2H_5)_2)_4$ with different x values

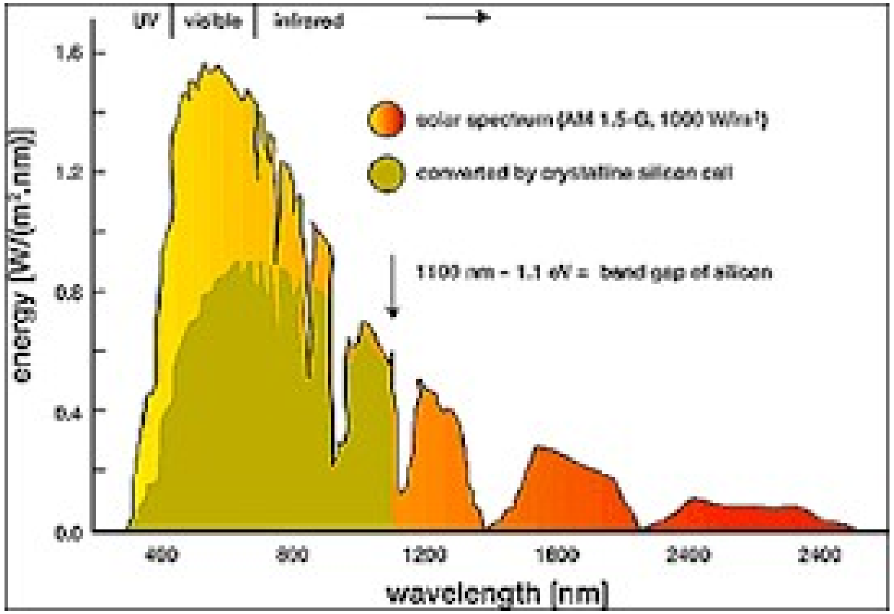
Si solar cells



A solar cell is a sandwich of n-type silicon (blue) and p-type silicon (red). It generates electricity by using sunlight to make electrons hop across the junction between the different flavors of silicon:

1. When sunlight shines on the cell, photons (light particles) bombard the upper surface.
2. The photons carry their energy down through the cell.
3. The photons give up their energy to electrons (green blobs) in the lower, p-type layer.
4. The electrons use this energy to jump across the barrier into the upper, n-type layer and escape out into the circuit.
5. Flowing around the circuit, the electrons make the lamp light up.

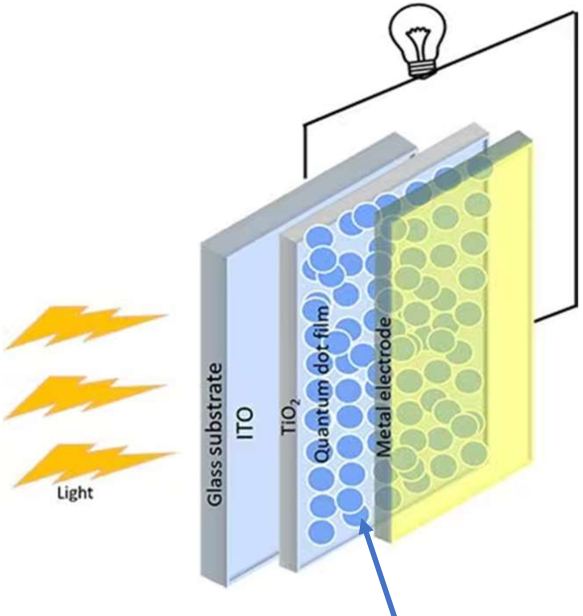
Si solar cells : performances



Solar cell efficiencies vary from **6% for amorphous silicon-based solar cells to 44.0% with multiple-junction production cells and 44.4% with multiple dies assembled into a hybrid package**.

Solar cell energy conversion efficiencies for commercially available multicrystalline Si solar cells are around 14–19%.

Quantum dots-sensitized solar cells

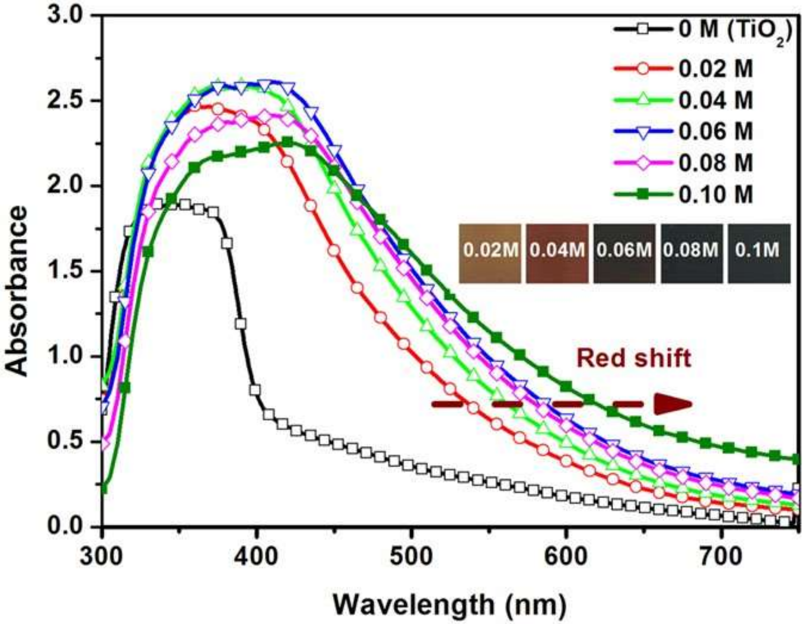


Quantum dots

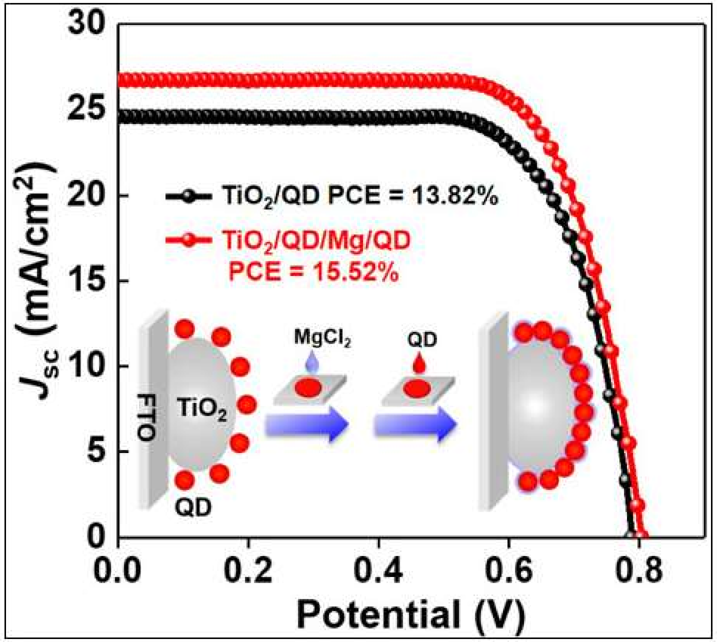
For PV cell applications, QDs must meet the following criteria to avoid a sharp deterioration in performance:

- QDs should exhibit a narrow bandgap allowing to harvest light in the visible and NIR region,
- The CB energy of QDs should be high to efficiency extract and transfer photogenerated electrons from QDs to TiO_2. A large difference of energy between the CB of QDs and that of TiO_2 promotes a fast extraction rate of photo-generated electrons,
- The density of defect trap states, especially deep-level trap states, should be low as these defects will not only cause a quenching of photo-excited electrons before their transfer to TiO_2 but also a back transfer of these electrons from TiO_2 which causes the charge recombination loss.

Quantum dots-sensitized solar cells

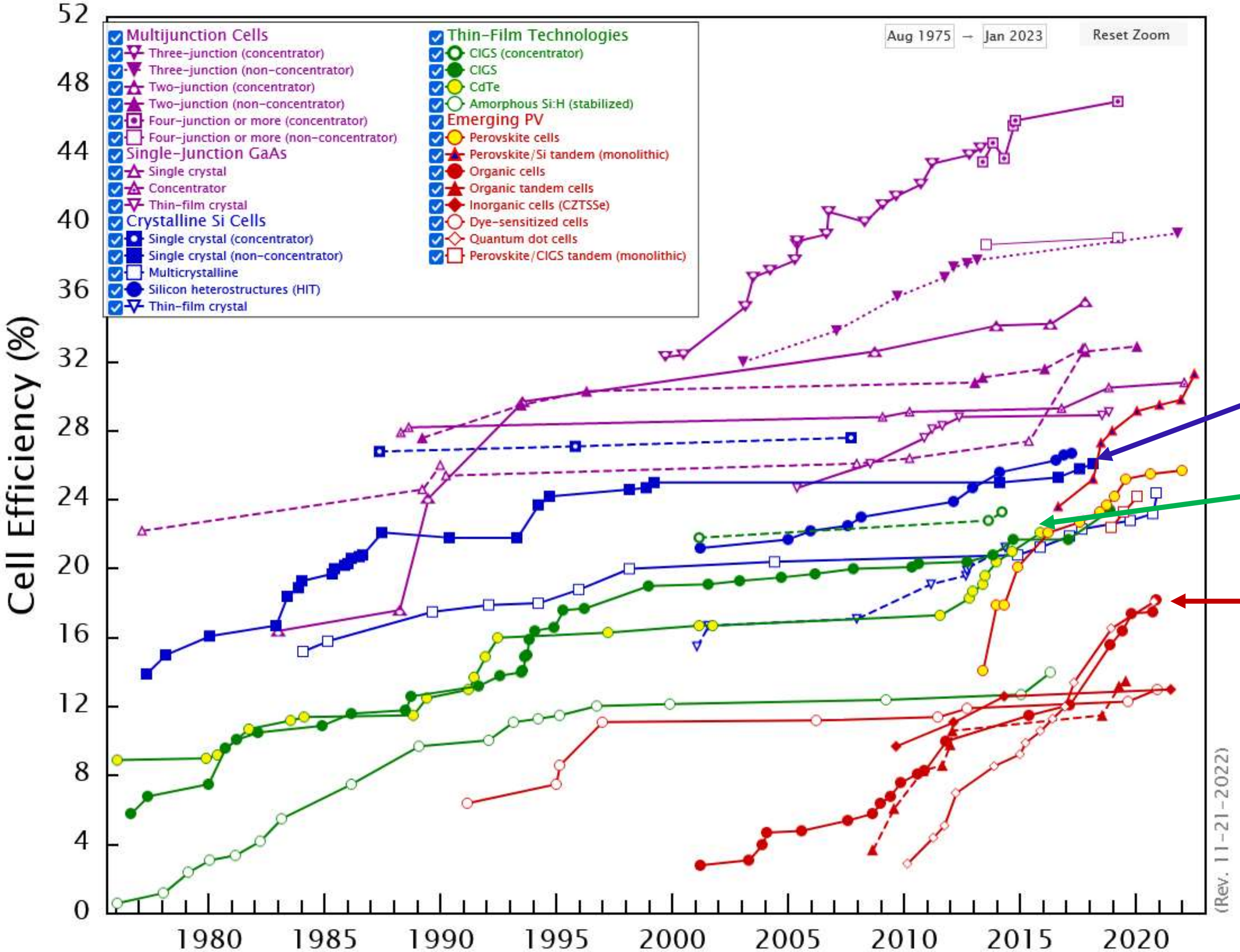


Recent reports show that the density of defect trap states in these nanocrystals can be controlled and decreased by tuning their chemical composition, for example by cation and/or anion alloying, which is key parameter for the optimal electron transfer in QDSSCs.



Moreover, **due to their large absorption coefficients and high conduction band energy**, I-III-VI_2 QDs were demonstrated to be of high potential for QDSSCs. **The highest PCE value reported to date is of 15.20% for Cu-In-Zn-Se-S QDs.**

Performances



A chart of the highest confirmed conversion efficiencies for research cells for a range of photovoltaic technologies, plotted from 1976 to the present.

Si cell

Cu-In-Ga-S

Quantum dots cells

Conclusion

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The performance of QDSSCs and the PCE still require to be improved.

This could be achieved by:

- Further **improving the light harvesting capacity of QDs** by the development of new materials,
- **Increasing the QDs loading on TiO_2**. This will allow to decrease the thickness of the QDs-sensitized photoanode and thus improve the absorption of incident photons.

A decrease of the thickness of the photoanode will lead to a short transportation path of photo-generated electrons and thus limit undesirable charge recombination. Moreover, if only a small part of the TiO_2 film is not covered by the QDs, the probability of photogenerated electrons to be trapped by the redox couple in the electrolyte will also decrease and this will markedly improve the fill factor *FF* and thus the PCE of the QDSSCs.

THANK YOU

CONTACT US FOR MORE INFORMATION

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