

Interfacial structure and dynamics for PbS quantum dot solar cells

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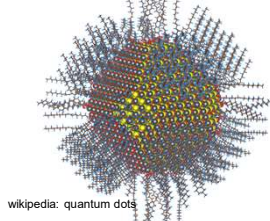


Background & Motivation

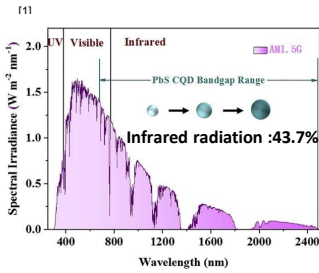
Device Architecture

Quantum dots

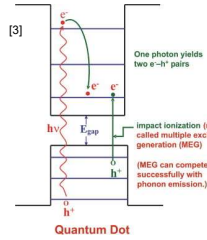
QDs' unique properties in solar cell



- artificial semiconductor NPs
- 2-10nm diameter

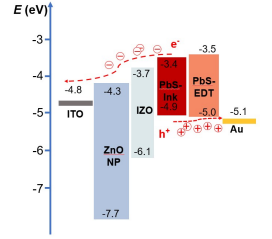
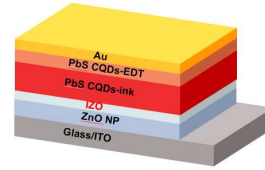


- Harvest infrared photons of the solar spectrum with QDs size dependent bandgap tunability



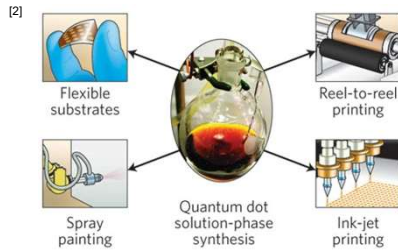
- Multiple exciton generation (MEG)

IZO as the buffering layer

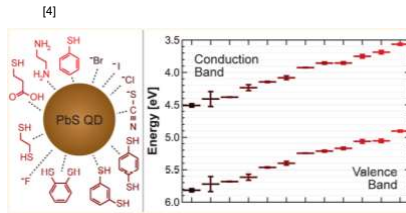


- Acquire the desired band alignment of IZO by tuning its thickness
- Reduce charge recombination and enhance charge extraction at PbS QDs/ZnO NP interface
- Inject and transport electrons more efficiently

Colloidal PbS QD Ink

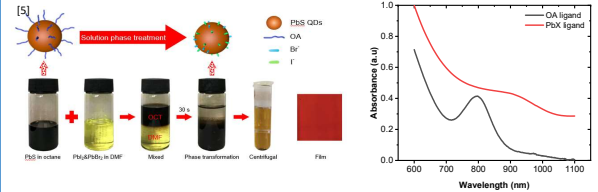


- Solution processibility



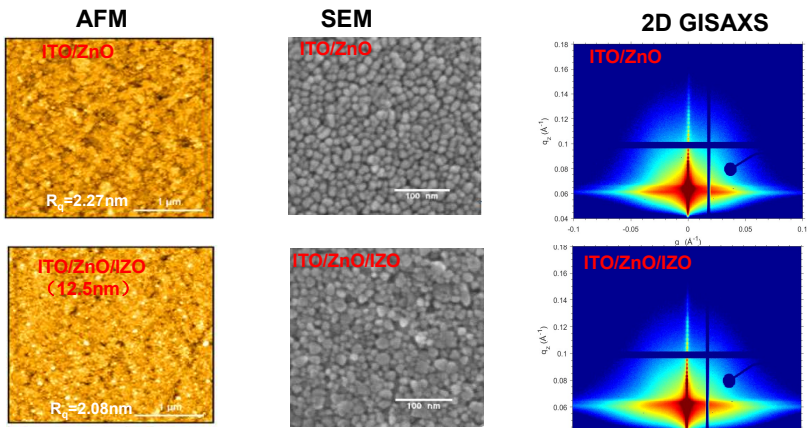
- Tune the property of QDs with variable surface treatment

Colloidal QD ink preparation



- Remove the surface ligands more thoroughly
- Make the scalable production of infrared solar cell feasible
- The absorption spectra of PbS QDs with short ligands shows red shifted and broadened exciton peak, which can be attributed to the decreased QDs' inter distance or their oxidation and less organization.

Morphology Characterization

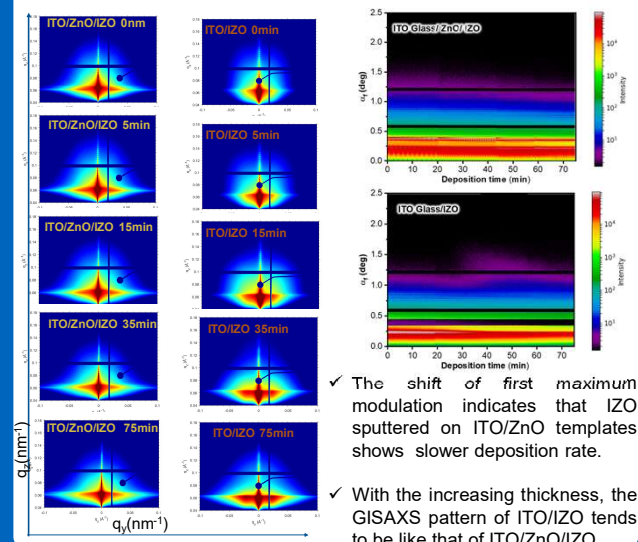


- The indium doped ZnO (IZO) film has higher roughness
- The grain size become larger and less even size distribution; the film on average is less densely packed
- The small difference in the 2D GISAXS data between ITO/ZnO/IZO and ITO/ZnO shows that the IZO layer grows conformally on the substrate surface

Conclusion & Outlook

- Colloidal QDs ink shows great potential for large scale fabrication, while the ink stability, trap density and related devices performance need to be further promoted
- In situ GISAXS during sputter deposition is a very powerful method
- The solvent engineering for QDs ink and ligands type for solution ligand exchange need to be explored more for optoelectronic devices applications

Interface Characterization



- The shift of first maximum modulation indicates that IZO sputtered on ITO/ZnO templates shows slower deposition rate.

- With the increasing thickness, the GISAXS pattern of ITO/IZO tends to be like that of ITO/ZnO/IZO



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[1] Zheng, Siyu, et al. *Science* 23.11 (2020): 101753.
[2] Sargent, Edward H. *Nature photonics* 6.3 (2012): 133-135
[3] Nozik, Arthur J. *Chemical Physics Letters* 457.1-3 (2008): 3-11.
[4] Brown, Patrick R., et al. *ACS nano* 8.6 (2014): 5863-5872.
[5] Marus, M., et al. *Applied Physics Letters* 116.19 (2020): 191103.

