The Road to Air-Stable Quantum Dot Solar Cells by Way of *1,4-phenylene-bis(dithiocarbamate)*

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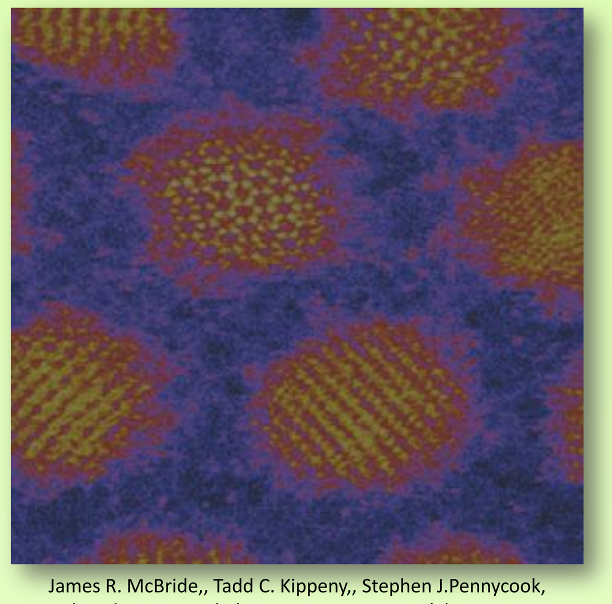
Introduction

In an effort to design a more low cost, highly efficient alternative to the traditional silicon solar cell, our research implements lead sulfide nanocrystals as light harvesters. Semiconducting nanocrystals are promising candidates for photovoltaics because they offer size-tunable band gaps, notably high extinction coefficients, and facile colloidal synthesis. Traditionally, however, nanocrystals suffer from high amounts of photo-oxidation and electron-hole-pair recombination.



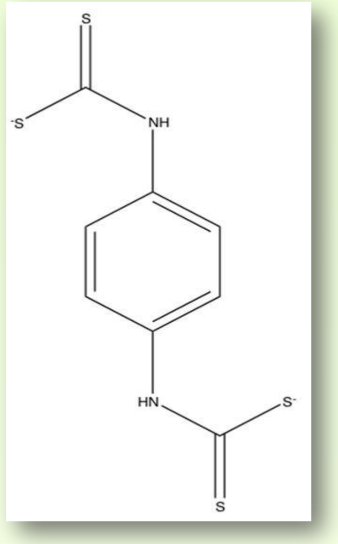
James R. McBride,, Tadd C. Kippeny,, Stephen J.Pennycook, andSandra J. Rosenthal. *Nano Letters 2004 4 (7), 1279-1283*

In light of this, *1,4-phenylene-bis(dithiocarbamate)* (PBDT) is investigated as a possible ligating species that has promise of not only facilitating electron transport due to being fully conjugated, this ligand should also fully passivate the surface of the nanocrystals. Theoretically, this full passivation would render the nanocrystal more resilient to photo-oxidative effects, leading to more air stable devices. In this study, devices are tested routinely over a period of several weeks to monitor the effect that PBDT has on the lead sulfide nanocrystals

PBDT Synthesis

PBDT was synthesized according to a modified procedure by Wessels, *et al.*

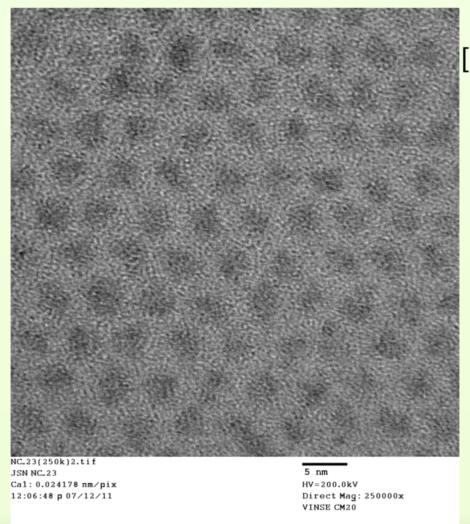
1. 100-mL H_20, 5.0-g NaOH, and 5.4-g p-phenylendiamine heated to 55°C until dissolved.
2. Cooled to <10°C and 7.25-g CS_2 added dropwise.
3. Slowly heated to 60°C for 2 hours.
4. Cooled to RT and poured into 2.5-L acetone.
5. After 30 minutes an off green crystal powder was filtered and washed with acetone and dried under a vacuum.



PbS Nanocrystal Synthesis

Nanocrystal synthesis is carried out in an inert atmosphere with degassed and dried solvents and precursors.

1. 0.45-g PbO, 18 mL ODE, and 1.5 mL oleic acid put under vacuum and heated to 95° C, leaving lead oleate.
2. 10 mL ODE heated separately to 80°C and put under vacuum.
3. 290 μL TMS injected into the 80° ODE.
4. Lead oleate was heated to 120°C and immediately the ODE and TMS were injected.
5. Let cool to 60°C and then cleaned up with acetone and toluene washes followed by centrifugation to remove excess organics.



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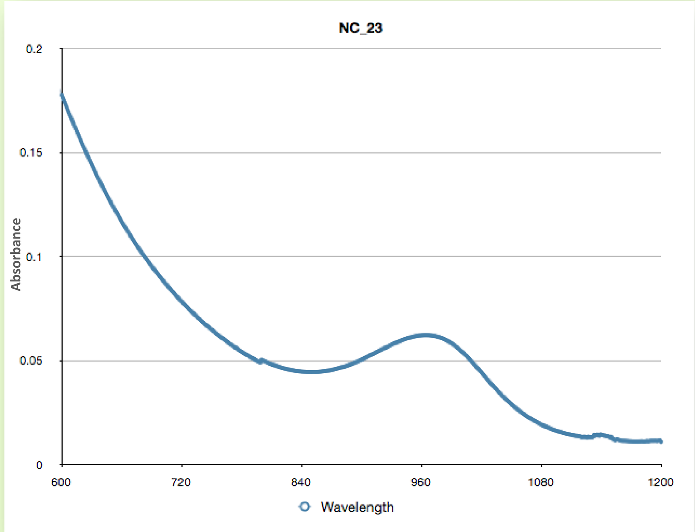

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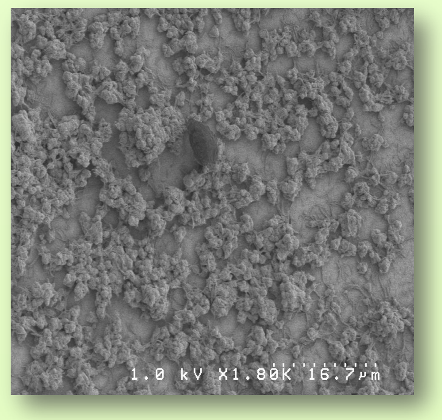
[1] Low resolution TEM of NC_23.
[2] UV-Vis-IR spectrum of NC_23.

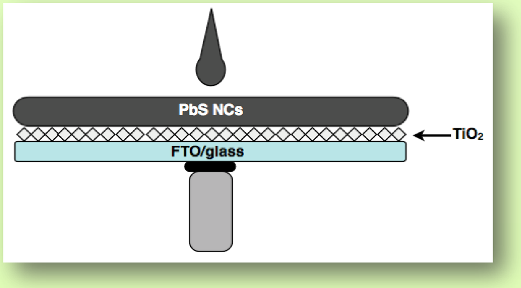
TiO_2 Electrode Preparation

TiO_2 paste is prepared using Hombikat TiO_2 nanoparticles and titanium isopropoxide. Paste is spin-cast onto a substrate of SnO_2:F (FTO) on glass at 3000 RPM for 60 seconds. Electrodes are then annealed in a glass tube furnace at 450°C for one hour.



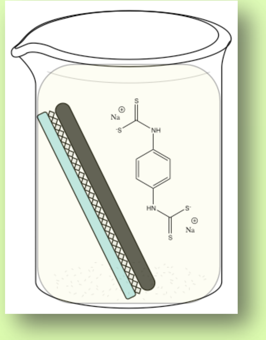
SEM of TiO2 on FTO substrate.

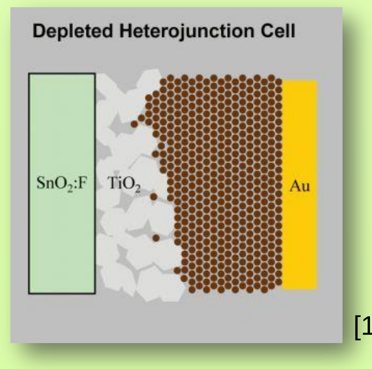
Device Fabrication



• Photovoltaic devices are prepared by spinning a TiO_2 electrode while dropping the PbS nanocrystals onto the substrate.

• Once the nanocrystal are applied, the device is dipped into a beaker filled with the PBDT ligand. The excess organics are washed away and the process is repeated approximately ten times.





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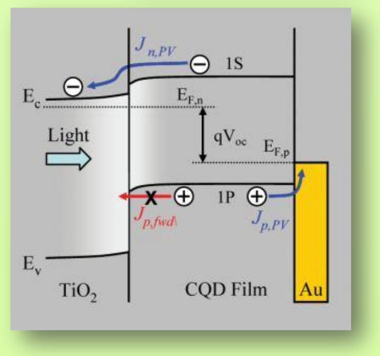
• Gold is then evaporated onto the nanocrystal surface to act as a cathode. Giving us our end product.



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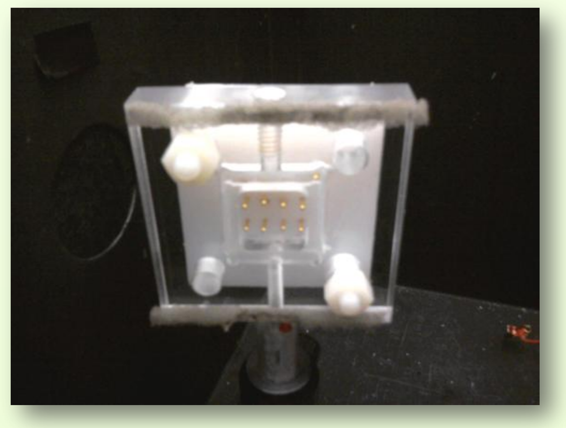
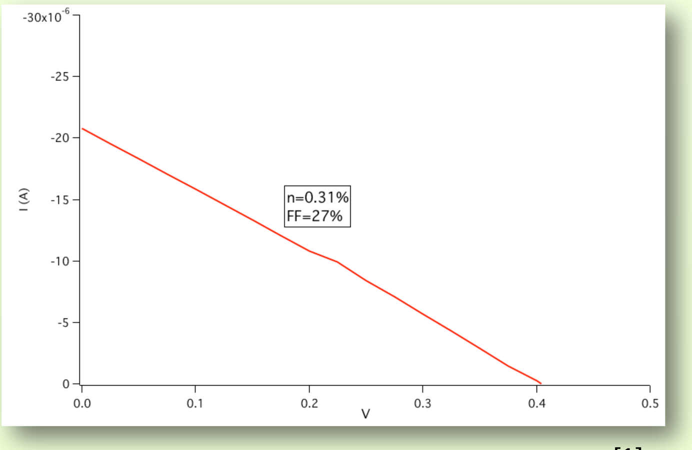
[1] Cross-sectional representation of device.
[2] Band diagram of device.
Sargeant *et al*. ACS Nano 2010 4(6), 3374-3380

Testing and Results



• Efficiency tests are carried out with a device which holds each sample and has electrical probes which contact the Au cathodes.

• As these test are still in the preliminary stages, our champion device thus far, which consists of both PBDT and MPA ligands shows an initial efficiency of 0.31%.



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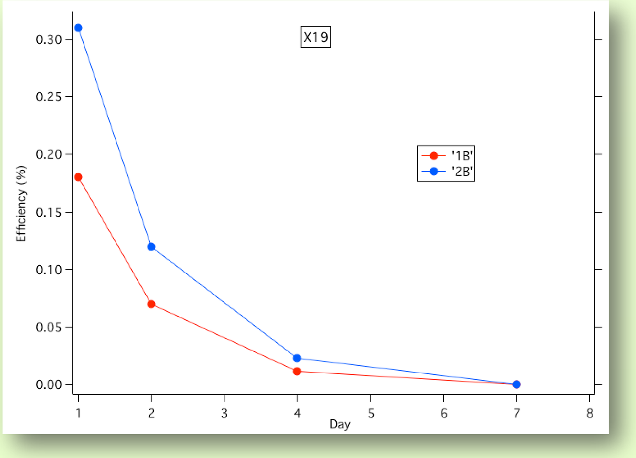

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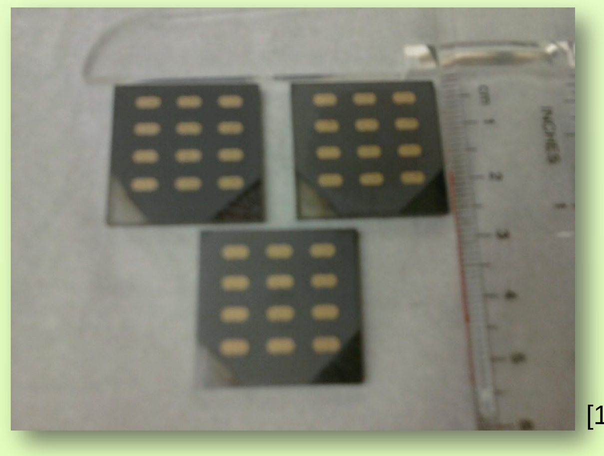
• After testing this control device over a period of one week, the efficiency is seen to suffer over time due to the effects of oxidation.

[1] I-V curve for sample X19
[2] Efficiency v. time graph for sample X19.

Future Goals

Our future plans are to make devices using strictly PBDT and measure the air-stability and compare them to devices which have not been passivated by their ligands. These devices promise equal or higher efficiencies which are more robust and resilient to the effects of oxidation.



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[1] Image of completed devices.

Acknowledgements

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