**BAPVC Annual Project Report**

**Project Title:** Applying Cation-Exchange Chemistry to Nanowire Arrays for Efficient Solution-Processed Solar Cells

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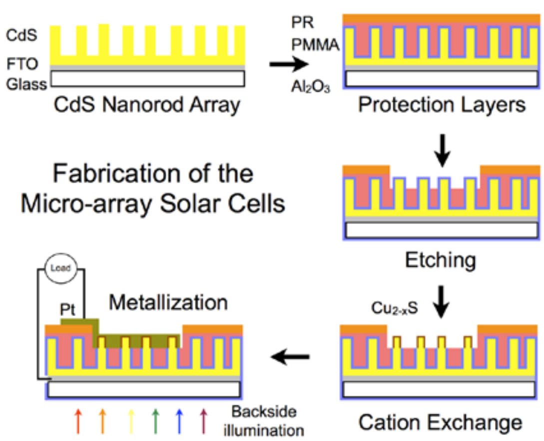
**Summary:**

This group is developing solution-processed sulfide-based nanowire array solar cells that take advantage of improved charge collection and light-trapping effects in nanowire arrays. Previously, this group used a cation-exchange reaction to form core-shell, CdS-$Cu_2S$ single-nanowire solar cells with excellent fill factor (~81%) and $V_{OC}$ (>0.6V).[1] Within the past year, this group has developed the ability to make working CdS-$Cu_xS$ core-shell nanorod array solar cells, and this group has also initiated efforts to model these solar cells.

**Key Accomplishments:**

In the past year, this group has synthesized CdS nanorod arrays on conductive fluorine-doped tin oxide (FTO) substrates through a hydrothermal method, which can be used as substrate for the creation of CdS-$Cu_xS$ core-shell nanowire solar cells. As shown in figure 1, after protection layers are added to prevent shorting of the p-type $Cu_xS$ to the n-type contact, the CdS nanorod array can be dipped into an aqueous $Cu^+$ solution to perform cation exchange to yield an array of CdS-$Cu_xS$ core-shell nanorods. The phase and thickness of the $Cu_xS$ can be controlled by varying the cation exchange temperature and time. While optimization of the devices is still ongoing, the initial devices exhibit a photoresponse. A plot of the I-V characteristics of one initial device is shown in figure 2.

1.




2.

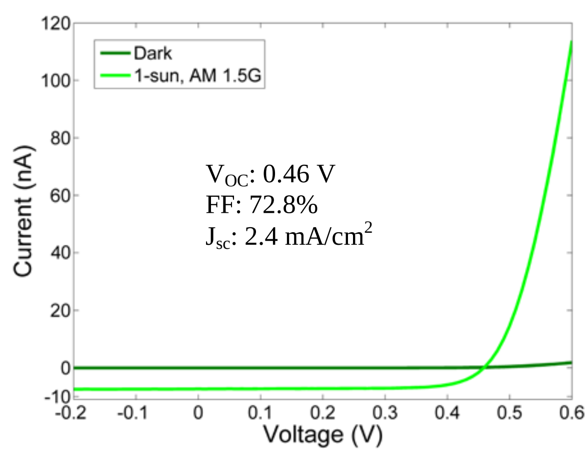



**Fig. 1** Schematic for the fabrication of the CdS-$Cu_xS$ core-shell nanorod array solar cells.
**Fig. 2** Plot of IV characteristics of an initial nanorod array solar cell 16 x 16 µm in area.

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[1] Tang, J., et al. *Nature Nanotech.* 6, 568 (2011).

Work is underway to model the CdS/$Cu_2S$ heterojunction and the performance of the nanorod array solar cell following previous reports. The description of the CdS/$Cu_2S$ heterojunction is carried out by a pseudospectral method that can calculate electronic energies, electron densities, wavefunctions, and band-bending diagrams while accounting for local and nonlocal electronic effects.[2] After coding the program, an example plot of the electron density in a CdS-$Cu_2S$ core-shell nanorod is shown in figure 3. With this data, it will be possible to calculate the effect of variables such as nanorod radius, length, and carrier concentration on the efficiency of a photovoltaic device systematically as has been demonstrated with homojunction nanorod solar cells.[3]

3.

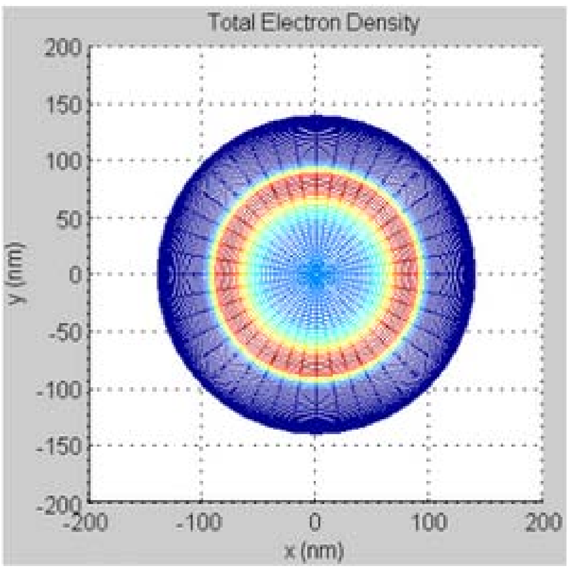


**Fig. 3** Plot of electron density in CdS-$Cu_2S$ core-shell nanorod. The carrier concentration of the $Cu_2S$ and CdS are fixed at $10^{19}$ and $10^{17}$ $cm^{-3}$ respectively while the core CdS has a diameter of 150 nm.

**Future Work:**

Future work will build on the successful fabrication of a nanowire array photovoltaic devices. This group will optimize performance by controlling the chemistry of the formation of the p-n junction, the geometry of the nanowire array, and the design of the electrical contacts to improve short circuit current density.

[2] Long, A.W.; Wong, B.M. *AIP Advances*. 2, 32173 (2012).
[3] Kayes, B.M.; Atwater, H.A. J. Appl. Phys. 97, 114302 (2005).