

Ligand Exchange Treatments in PbS Quantum Dot Solar Cells

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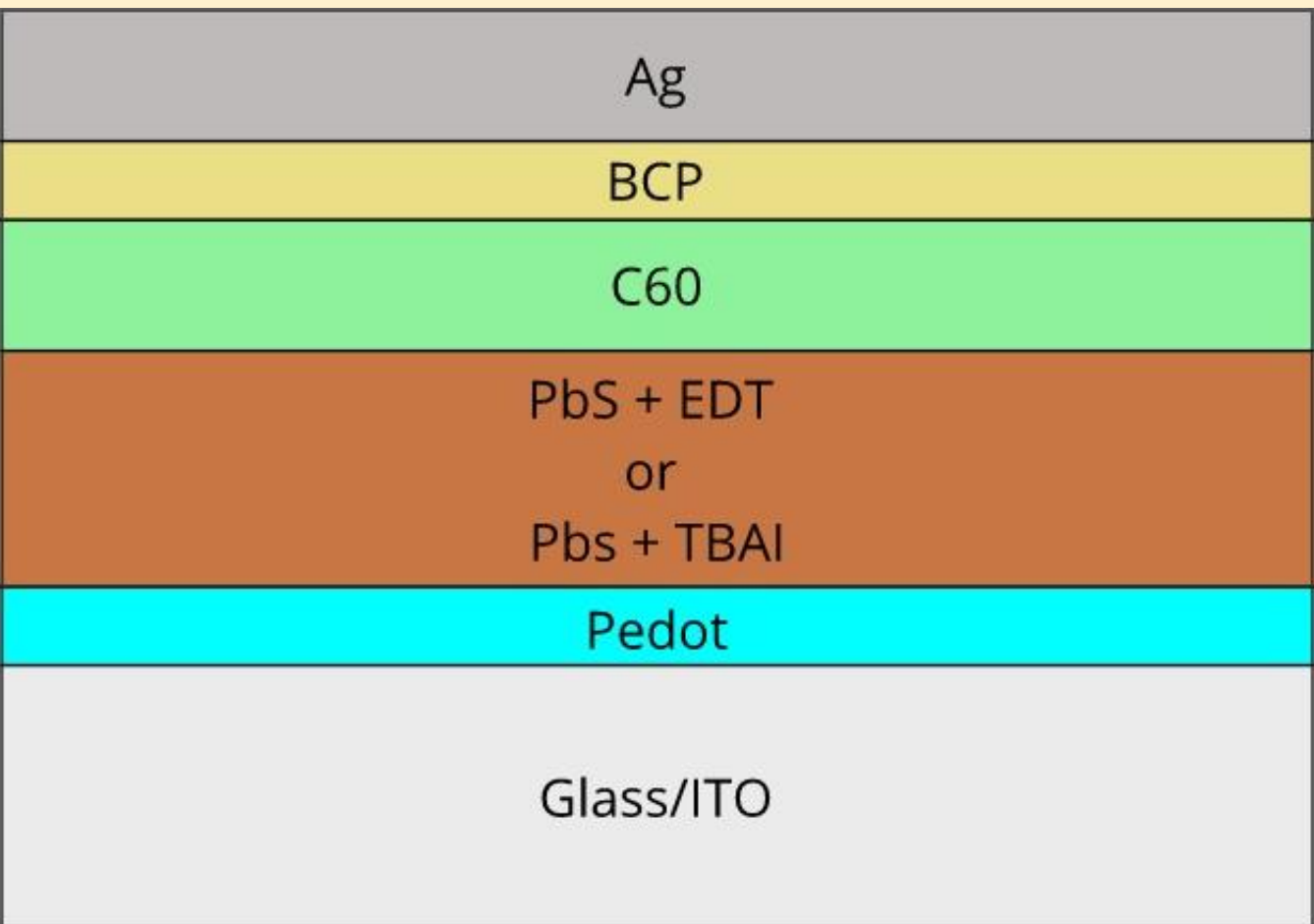
BACKGROUND

- Lead-sulfide (PbS) quantum dots (QDs) are attractive materials for developing the next generation of solar cells due to their low-cost fabrication.
- A quantum dot is a semiconductor particle that’s only several nanometers in diameter.
- One of the barriers to higher efficiencies and to generate a desired open circuit voltage is the presence of trap states.
- A trap state is a location within a solid that restricts the movement of charge. Having fewer trap states in these devices is crucial to their performance.
- PbS quantum dots are surrounded by long ligands that hinder the movement of charge between the dots, resulting in fewer trap states.
- During the spin coating process, PbS films undergo a ligand exchange treatment that replaces the longer ligands found in the PbS solution with shorter ligands found in the chemical they’re treated with.
- Replacing the longer ligands from the PbS solution with shorter ligands brings the QDs closer together in the film, allowing for better conductivity. This should also help increase the open-circuit voltage generated by the device.
- Changing the chemical used for the ligand exchange treatment will affect the amount of trap states in the device.

DEVICE STRUCTURE

The basic structure of the devices created for this experiment is:

- A clean glass substrate with ITO (Indium tin-oxide)
- One layer of pedot film is spun directly on the glass substrate to create a more even coat of PbS.
- PbS films are spin coated directly on top of the pedot film. These films can vary in number of layers and thicknesses.
 - Each layer of PbS film is treated with chemical that swaps the longer ligands found in the PbS solution with shorter ligands.
 - Each layer is also given a wash to clean off any excess ligands from the surface.
- A C60 film 36nm to 40nm thick is deposited on top of the PbS film.
- A BCP film 4nm to 10nm thick is deposited on top of the C60 film.
- Ag electrodes 60nm to 80nm are deposited on the very top of the device.



EXPERIMENTING WITH EDT AND TBAI LIGAND TREATMENTS

Post-Anneal Treatments

Process:

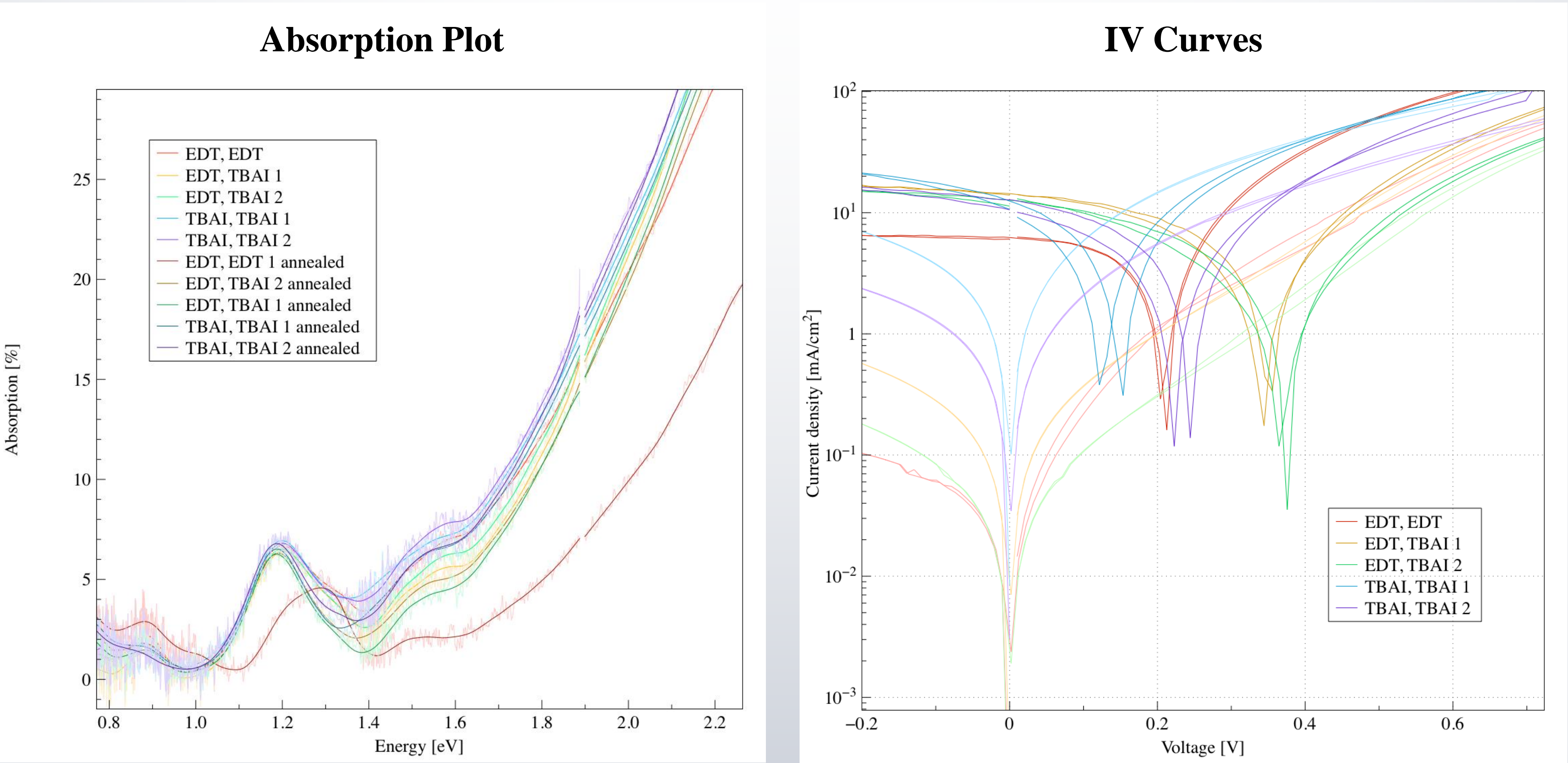
- Two films that were already spin coated with the same process were used. Both films were treated with EDT during the spin coating process.
- Both films were annealed at 115 degrees C for 30 minutes.
- After annealing, one of the films was treated with EDT and the other film was treated with TBAI.

Spin Coating and Post-Anneal Treatments

Process:

- Five two-layer PbS films were created using the spin coater with different ligand treatments:
 - One device where both PbS layers are treated with EDT (this is the control device).
 - Two devices where the bottom PbS layer is treated with EDT and the top PbS layer is treated with TBAI.
 - Two devices where both PbS layers are treated with TBAI.
- All PbS films were annealed at 60 degrees C for 3 hours. The EDT-only device was treated with EDT after annealing, and the rest were treated with TBAI after annealing, since the top PbS layer was also treated with TBAI.
- 40nm of C60, 10nm of BCP, and 80nm of Ag was deposited on all of the devices using a thermal evaporator.

Because the devices with PbS/EDT + PbS/TBAI films had the best performance, the next step of this project will be to figure out how to get higher values for Rleak, and to get an eV shift in the absorption curves after annealing in these devices.

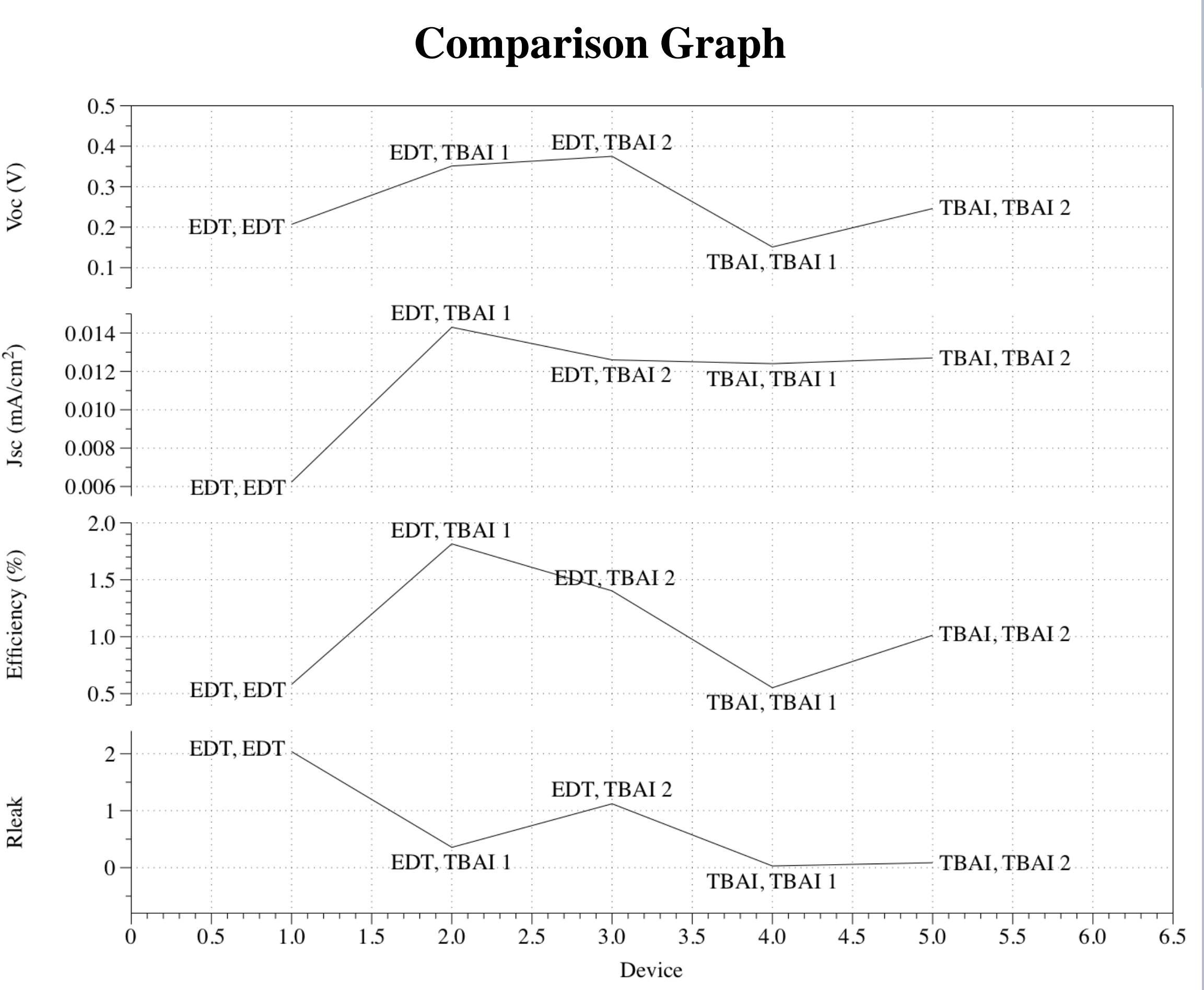


NEXT STEPS FOR THIS PROJECT

- The next steps of this project will be conducting more experiments in order to solve these problems occurring in the devices.
- Even though some useful information about ligand exchange treatments was obtained with these experiments, there’s still work to be done on this project.

The current stage of this ligand exchange treatment project is attempting to obtain a higher value of Rleak by creating thicker PbS films.

- New films will be fabricated by spin coating four layers of PbS rather than two.
- Since the number of PbS layers is being increased, an experiment needs to be conducted to figure out how many of these layers should be treated with EDT and how many should be treated with TBAI.
- Using thicker films should increase the values of Rleak, which should increase the performance of the device and help obtain a higher open-circuit voltage.
- Higher percentages on the absorption plot should be seen with thicker films.
- Higher short-circuit current should be seen with more absorption.



RESULTS

- Overall, the best performing devices from these experiments are those with PbS films treated with EDT on the bottom layer and TBAI on the top layer.
- Post-annealing treatments work best when they use the same ligand as the treatment of the top layer of the PbS film.
- The best open circuit voltage was 0.375 volts, which was found in a device treated with both EDT and TBAI. The worst open circuit voltage was found in a device treated with TBAI only.
- All devices treated with either EDT and TBAI or TBAI only show an improvement in the short-circuit current. The best short circuit current is $-1.43e^{-2}$ which is found in a device treated with both EDT and TBAI.
- The devices treated with both EDT and TBAI show the best efficiencies, with the highest efficiency being 1.815%.
- The only improvement we haven’t seen by adding TBAI in the PbS film treatment is the leakage resistance (Rleak). The best Rleak was 2.038, and was found in the device treated with EDT only.
- Problems occurring in these devices include low values for Rleak, and the fact that an eV shift in the absorption curves after annealing is not seen.