QUASI-TWO-DIMENSIONAL HALIDE PEROVSKITE MATERIALS FOR PHOTOVOLTAIC APPLICATIONS

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As energy demands for the world increase, the necessity for alternate sources of energy are critical. Just in the United States alone, 92 quadrillion British thermal units (Btu) were used in 2020. As political and geographical pressures surrounding oil increase, along with the growing concern for climate, the drive to explore alternative and renewable means for harvesting energy is on the rise. Solar cells, also known as photovoltaics (PVs), are an attractive renewable source and have been developed as an alternative energy means for over 60 years. When considering losses due to atmospheric absorption and scattering, the Earth's surface gets about 1000 W/m^2 of energy from the sun, which is why there are research efforts around the world trying to maximize the efficiency of solar cells.

Organic-inorganic halide perovskites provide for ideal absorbing layers that feature long carrier lifetime and diffusion lengths, strong photoluminescence, and promising tunability. Furthermore, the solution-processing methods used to make these perovskites ensure that the solar cells will remain low-cost and have easy scale-up possibilities. The main problem perovskites is that they degrade in the presence of water, thus leading to decreased device performance.

In this work two approaches are investigated to increase moisture stability. The first investigates incorporation of thiols as pseudohalides into the 2D perovskite structure. Instead of the theorized perovskite, two novel 2D compounds were created, $Pb_2X(S\text{-}C_6H_5)_3$ (X= I, Br, Cl) and $PbI_{1.524}(S\text{-}C_6H_5)_{0.476}$. While not perovskites, this study gives insight into the effect that the thiol may have on determining structure when comparing $–S\text{-}C_6H_5$ with –SCN groups. Future work will explore more electronegative thiols that will be used to make moisture resistant, tunable 2D perovskites.

The second approach is to incorporate longer organic ammonium cations into the perovskite structure to produce quasi-2D perovskite films fabricate them into devices. Adding in

electronically insulating ligands leads to a stricter requirement for vertically aligned 2D films and special care must be taken to have efficient charge collection. The current field has successfully incorporated short ligands such as butylammonium (BA) into PVs, however the extension to larger and more beneficially hydrophobic ligands has been very scarce. In this work, a novel solvent engineering system is developed to create vertically aligned quasi-2D perovskite absorbing layers based off of a bithiophene ligand (2T). These absorbing layers are then characterized and incorporated into efficient PV devices. Generalizations to solvent conditions related to ligand choice is discussed herein, creating deep insights into incorporating more conjugated ligands into devices.