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<th>Title</th>
<th>Air stable Cs2SnI6 sensitizers: synthesis, investigation of crystal structure and its optoelectronic properties</th>
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<td>Author(s)</td>
<td>Jamaludin, Nur Fadilah Bte</td>
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Despite reports of high efficiencies for organolead trihalide (CH3NH3PbI3) based solar cells, its commercialization remains hampered by the presence of soluble lead compounds. Attempts to replace atoms in the typical ABX3 structure, such as in CH3NH3SnI3 and CsSnI3, have resulted in perovskites with long term instability issues associated with phase transitions and ambient hydrolysis, driving the research to uncover lead-free, air-stable substitutes.

A type of molecular iodosalts, Cs2SnI6, exhibits air and moisture stability attributed to Sn +4 oxidation state, unlike the +2 in CH3NH3SnI3 and CsSnI3. These, coupled with its solubility in common laboratory solvents, makes it ideal for ambient processing. Recent report on hole transporting capability of the cubic structured Cs2SnI6 in solid state dye sensitized solar cell (DSSC) has motivated the synthesis and characterization of high purity Cs2SnI6 to assess its suitability as a light absorber.

Two synthesis techniques were employed in an attempt to obtain high purity Cs2SnI6, namely precipitation and melt (Fig.2). Precipitation

Cs2CO3 (s) + 2 HI (l) → 2 CsI (aq) + H2O (l) + CO2 (g)

Melt

2CsI (aq) + SnI4 (aq) → Cs2SnI6 (s)

As shown above (Fig.3), pure Cs2SnI6 was successfully synthesized using the precipitation method. XRD patterns from Cs2SnI6 thin films with DMF as solvent (Fig.4) showed linear relationship between CsI content and annealing temperature, implying a need for solvent engineering and annealing temperature optimization.

Homogeneity of film plays a crucial role in material characterization and device performance. This necessitates solvent engineering to obtain a well dispersed layer to ensure accuracy, reliability and reproducibility of data.

Solutions of Cs2SnI6 in DMF and DMF + HI resulted in films with poor surface coverage with large crystal formation (1-6 um) (Fig. 5). Presence of CsI in XRD patterns of these films also indicate possible degradation due to solute-solvent interaction (Fig. 6). High purity film with smaller crystal sizes (~700nm) and better coverage were attained with DMF and HI as solvents.

Low efficiencies observed is likely due to insufficient loading of perovskite in the mesoporous layer, as evidenced by incomplete penetration of the absorber in the screen printed cell leading to low currents. Infiltration of the perovskite for screen printed films can be improved through addition of valeric acid. Further optimization of blocking and absorber layers necessary to improve fill factor and current density respectively.

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**Device Fabrication and Testing**

Gold Electrode
Deposited by thermal evaporation

Spiro-OMeTAD (Li+ and TBP)
Deposited via spin coating

Cs2SnI6 absorber
Deposited via spin coating

FTO Glass
Substrate

<table>
<thead>
<tr>
<th>Screen printed</th>
<th>Spin coated</th>
<th>I sc (mA/cm²)</th>
<th>Voc (V)</th>
<th>Fill Factor (%)</th>
<th>Efficiency (%)</th>
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<tr>
<td>0.0777</td>
<td>0.0385</td>
<td>0.2047</td>
<td>0.3019</td>
<td>35.18</td>
<td>6.07</td>
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**Project Title:** Perovskite Solar Cells

**Supervisor:** Prof Subodh Gautam Mhaisalkar

**Category:** 2
**Student:** Nur Fadilah Bte Jamaludin

FYP-URECA Project ID: MSE14004

School of Materials Science and Engineering

**URECA Undergraduate Research Experience on CAmpus**