

Supporting Information

Dual Functional Hetero-anthracene Based Single Component Organic Ionic Conductors as Redox Mediator cum Light Harvester for Solid State Photoelectrochemical Cells

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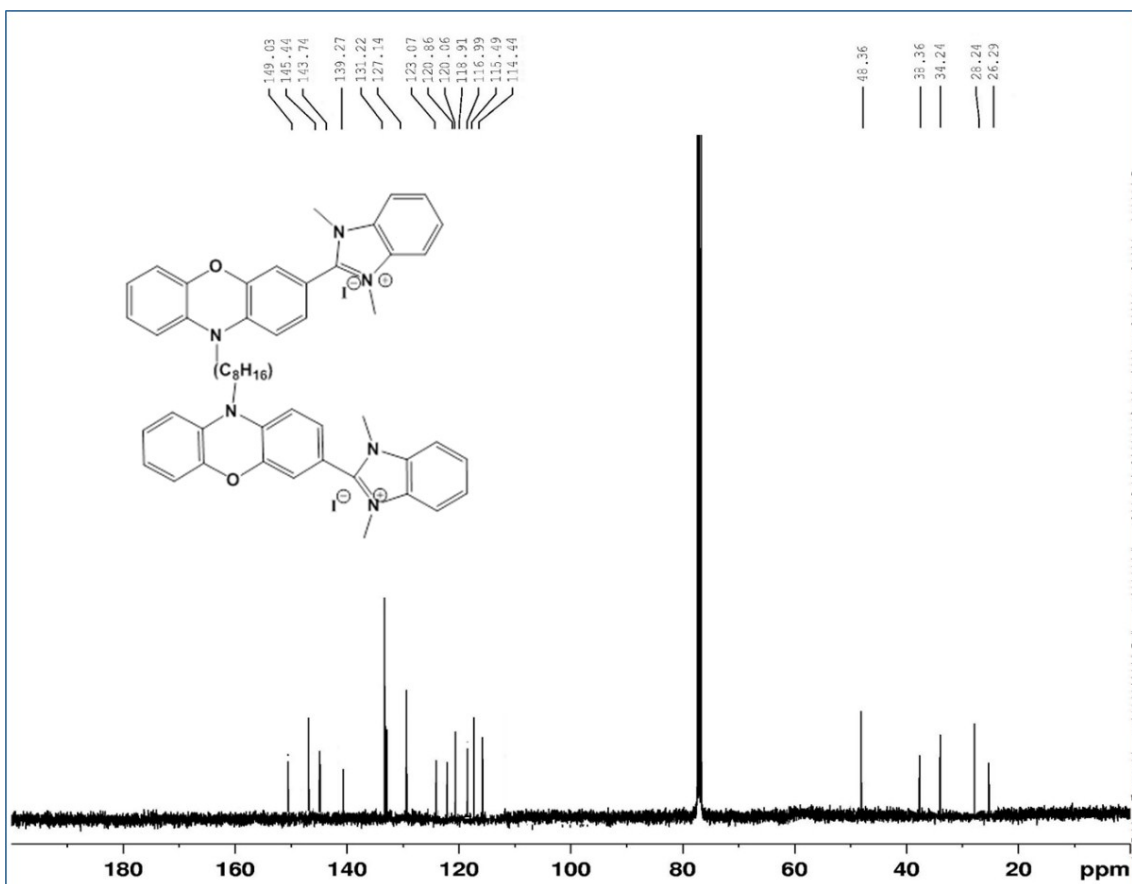
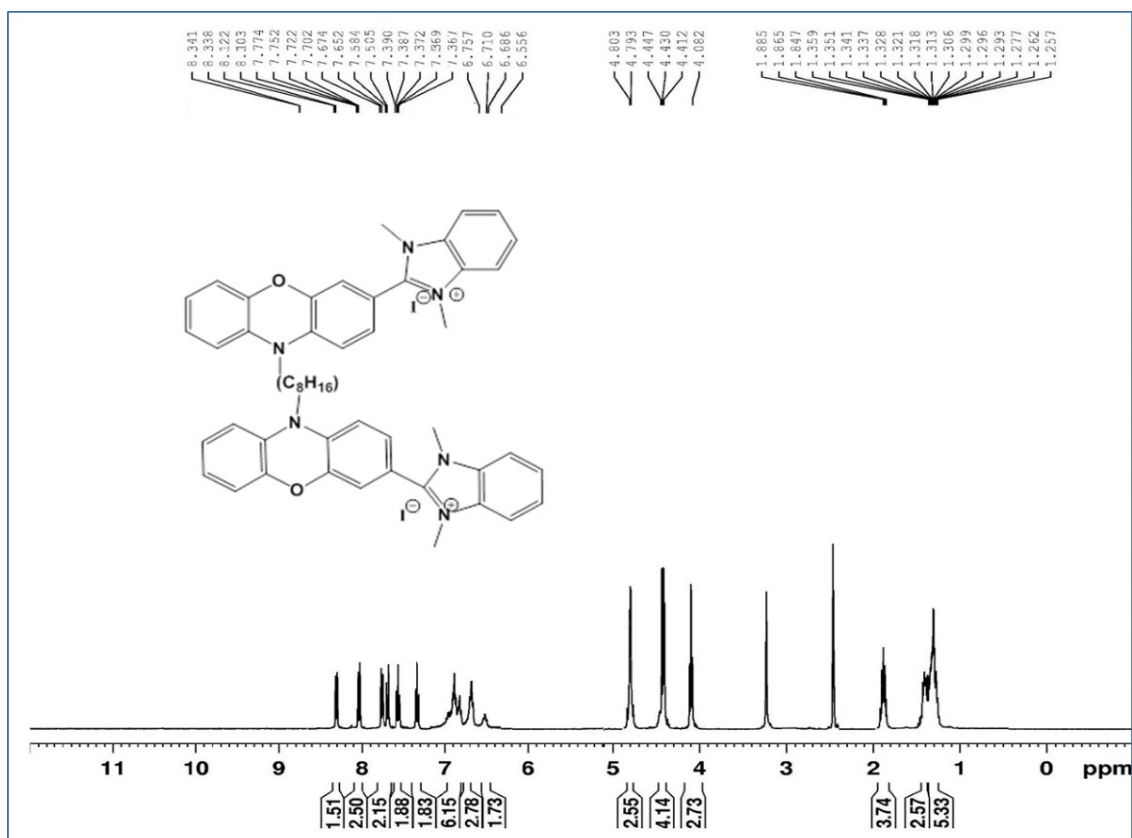


Fig. S1. ¹H and ¹³C NMR spectra of SOIC-1

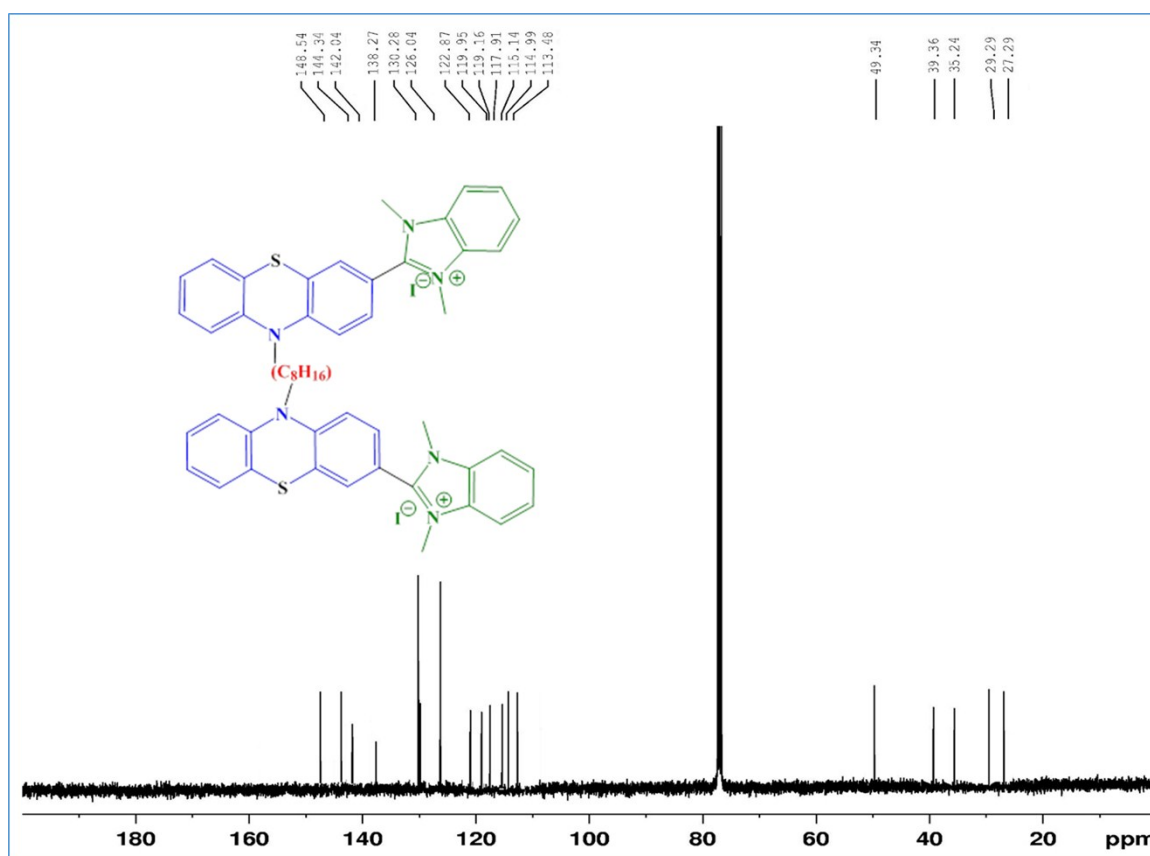
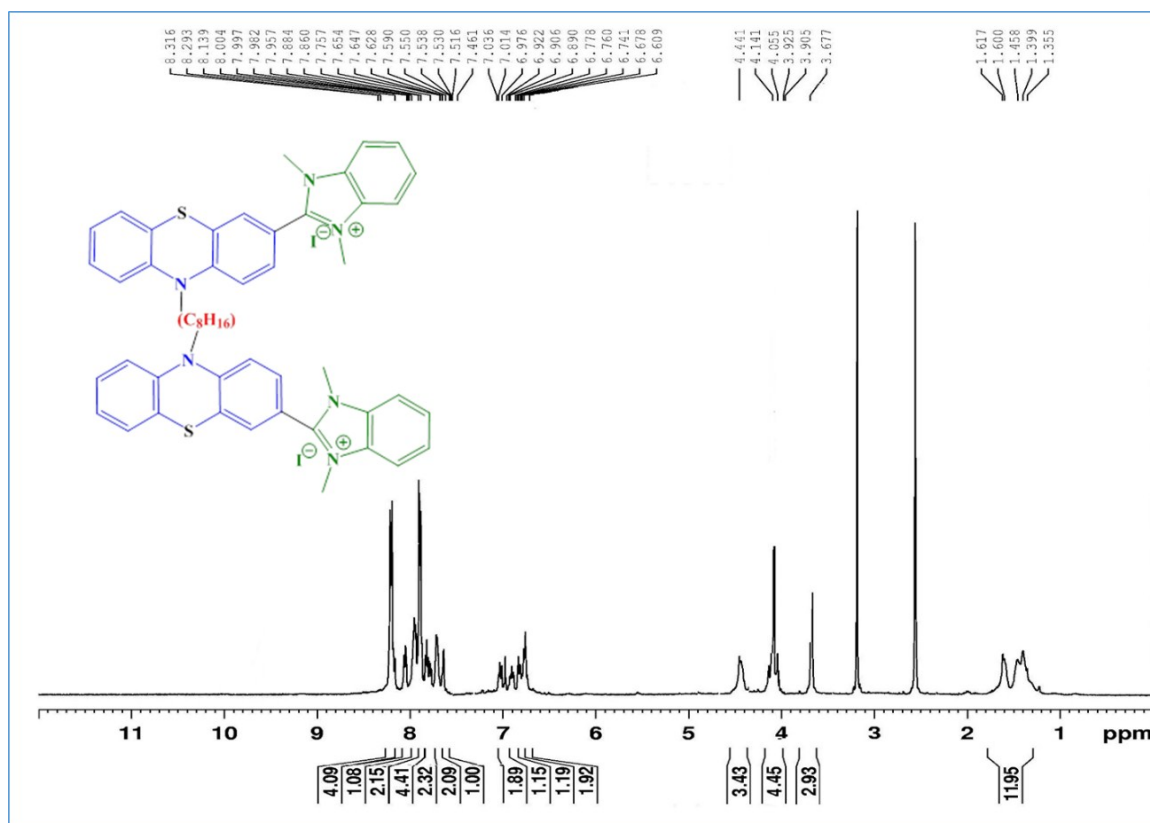
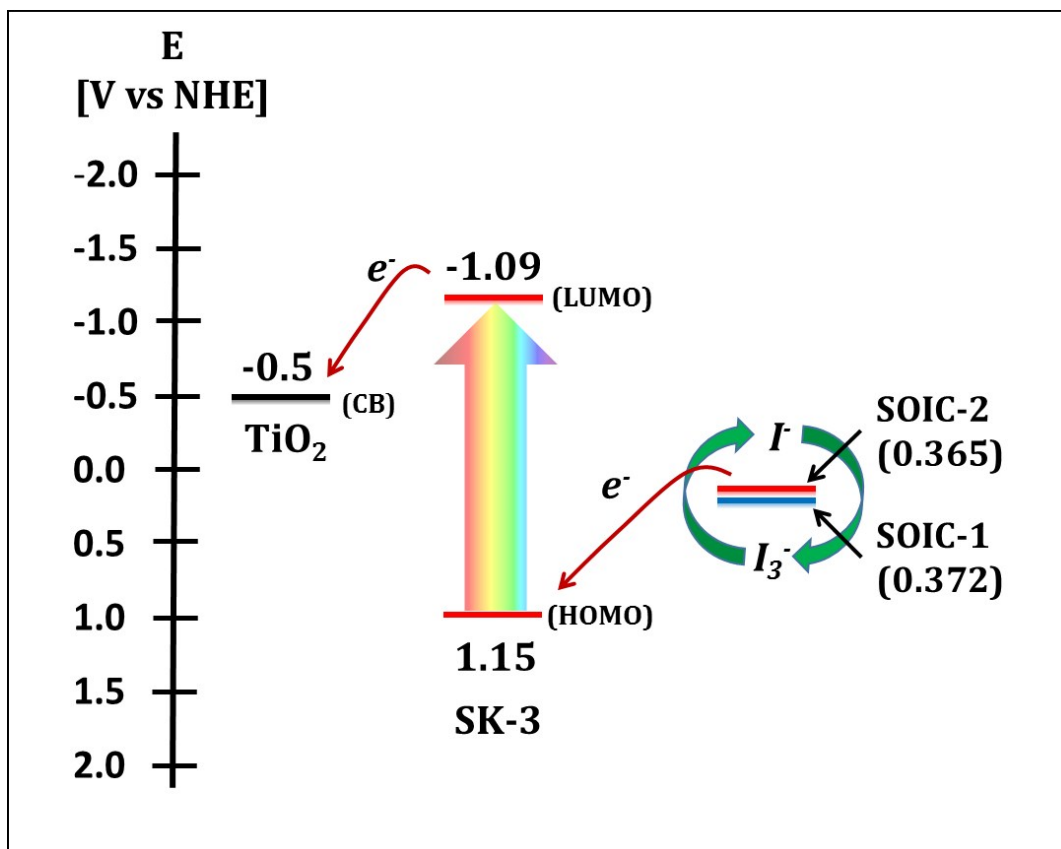


Fig. S2. ¹H and ¹³C NMR spectra of SOIC-2



Scheme S1. Energy level diagram of SOICs electrolyte based solid state photo-electrochemical cells.

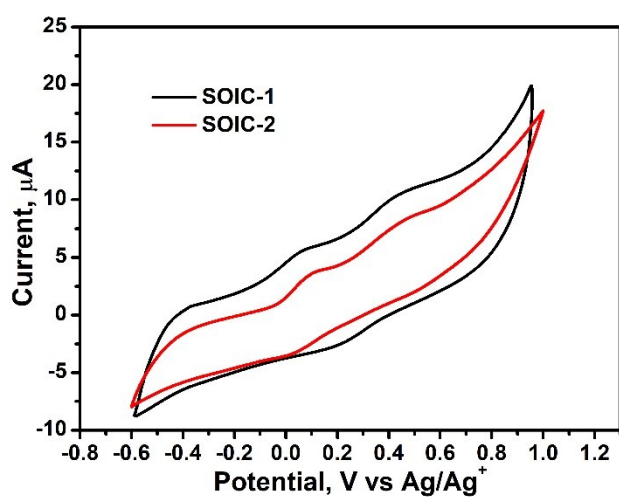


Fig. S3. Cyclic voltammetry was carried out using SK3 dye sensitized TiO₂ film as a working electrode.

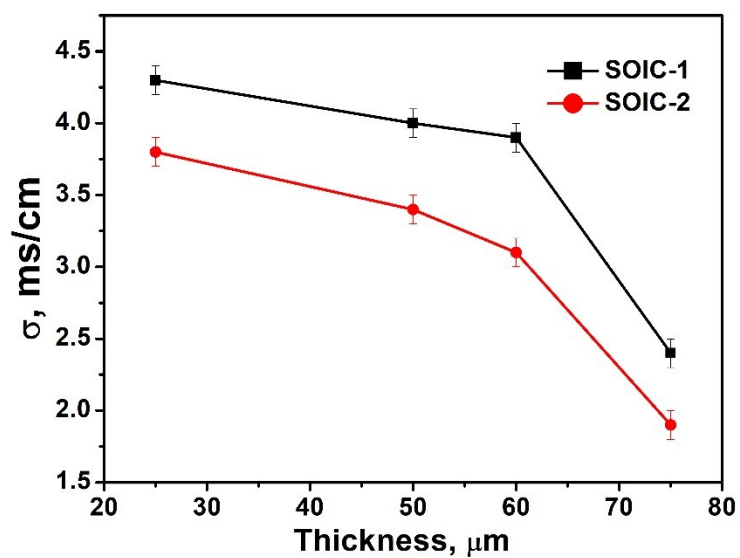


Fig. S4. Different thickness of SOICs vs conductivity at 25°C

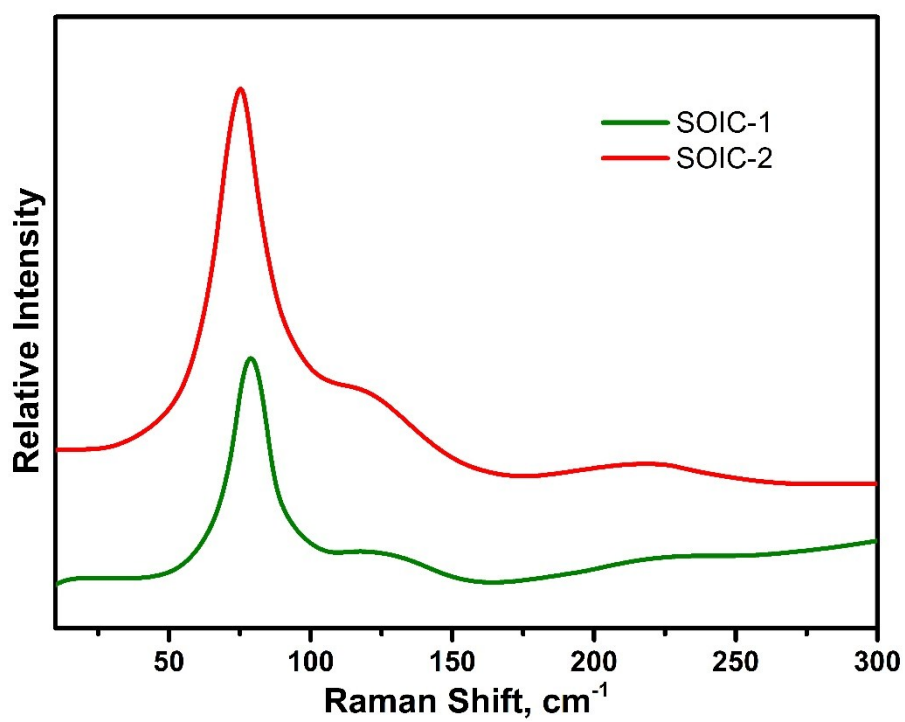


Fig. S5. Raman spectroscopy of SOIC-1 and 2.

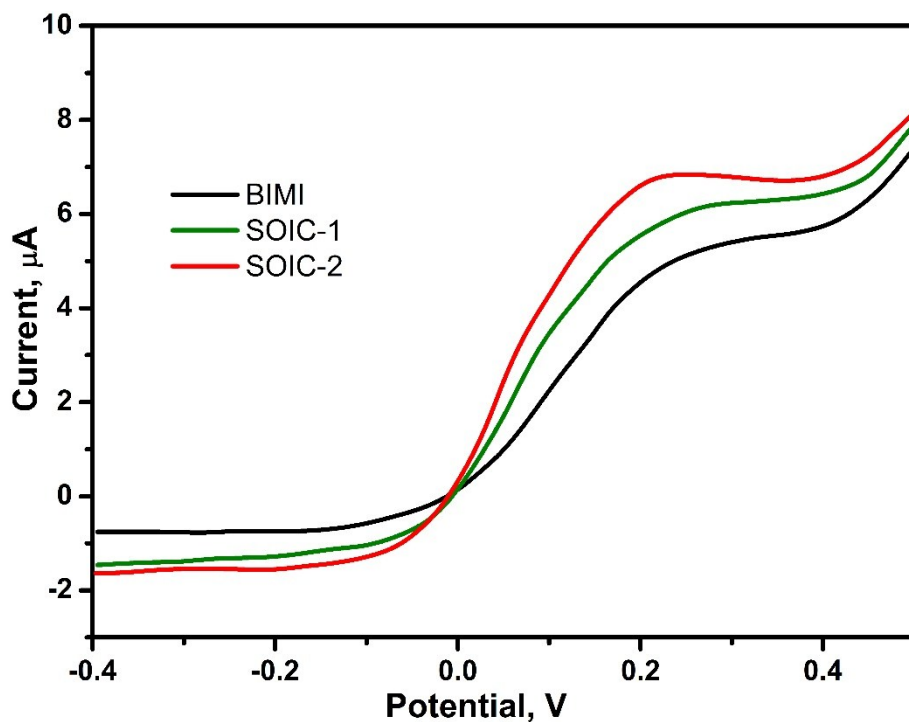


Fig. S6. Steady-state voltammety of SOICs and BIMI electrolyte

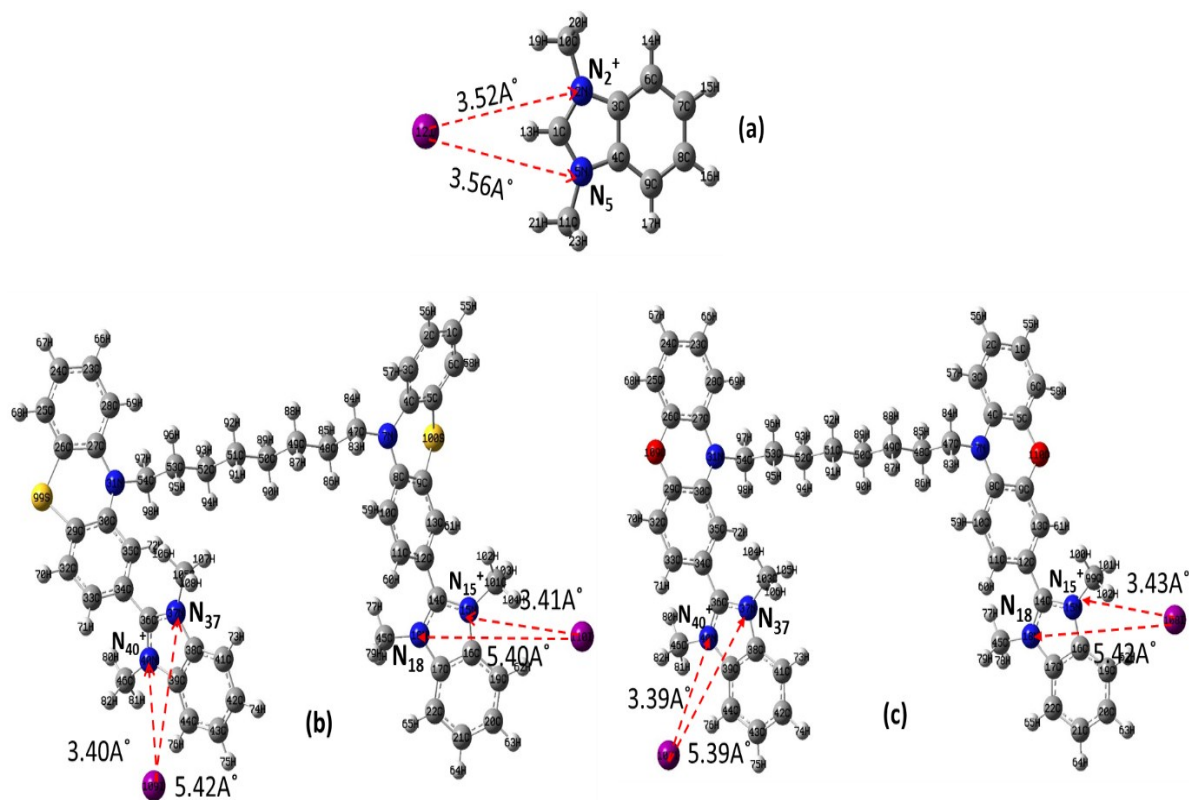


Fig. S7. Computationally optimized structure of (a) BIMI, (b) SOIC-1 and (c) SOIC-2.

Table S1. The optimized structure bond length of N-C, N-I, N-C-N and dihedral angles of BIMl cation with PTZ/POZ donor moieties (C13-C12-C14 and C35-C34-C36).

| Parameters | SOIC-1 (°A) | SOIC-2 (°A) |
|--------------|-------------|-------------|
| C14-N15 | 1.36 | 1.36 |
| C14-N18 | 1.36 | 1.36 |
| C36-N40 | 1.36 | 1.36 |
| C36-N37 | 1.36 | 1.36 |
| -C12-C14-N15 | 125.67 | 125.14 |
| -C34-C36-N37 | 125.89 | 125.16 |
| N15-C14-N18 | 108.59 | 107.60 |
| N37-C36-N40 | 108.78 | 108.20 |
| N15-I110 | 3.41 | 3.43 |
| N18-I110 | 5.40 | 5.42 |
| N40-I109 | 3.40 | 3.39 |
| N37-I109 | 5.42 | 5.39 |

Mulliken charge of BIMl

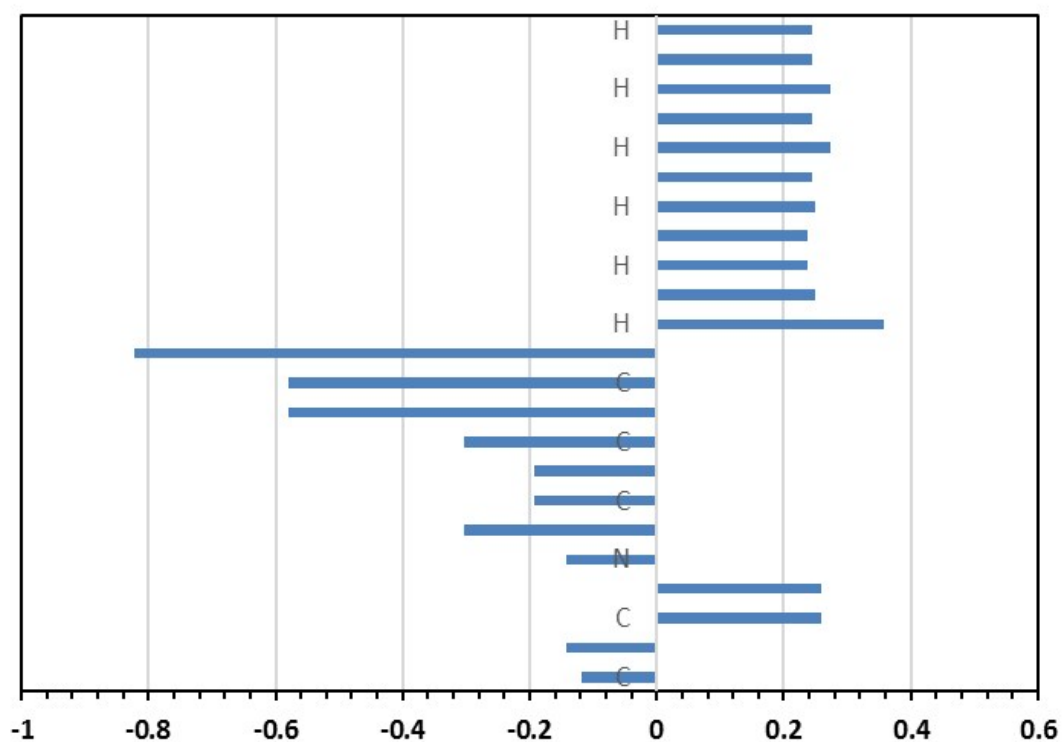


Fig. S8(a). Mulliken charge of BIMl

Mulliken charge of SOIC-1

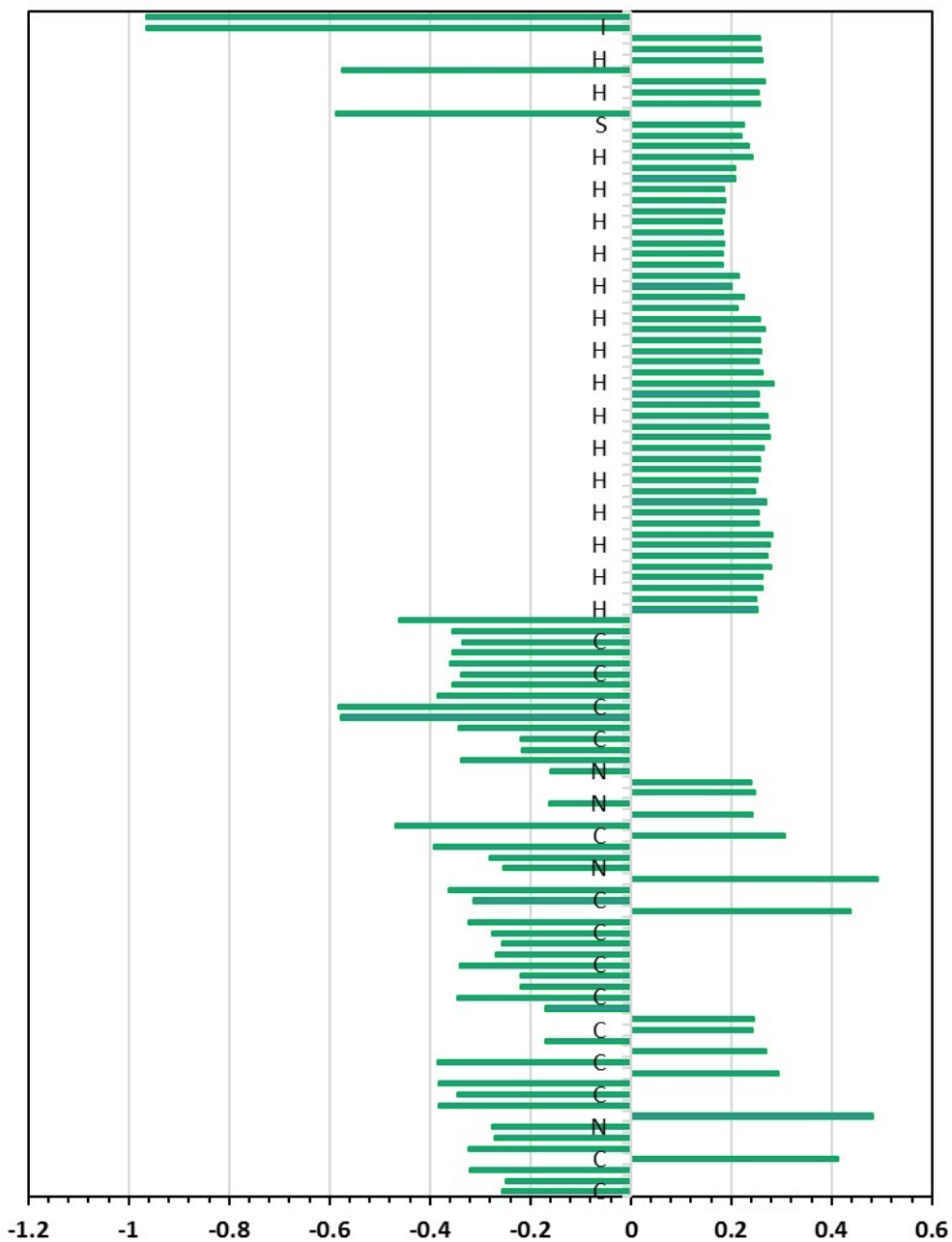


Fig. S8(b). Mulliken charge of SOIC-1

Mulliken charge of SOIC-2

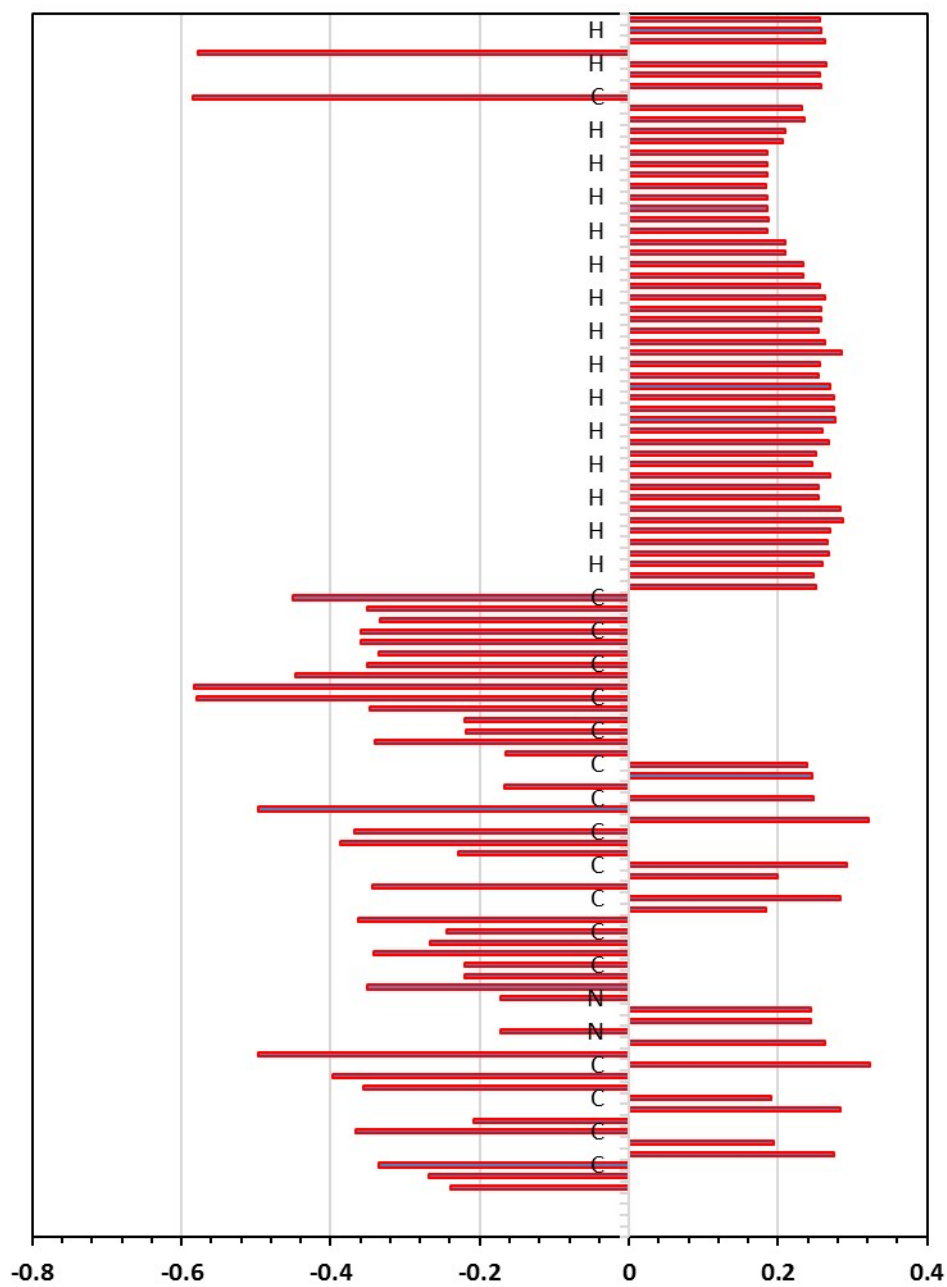


Fig. S8(c). Mulliken charge of SOIC-2

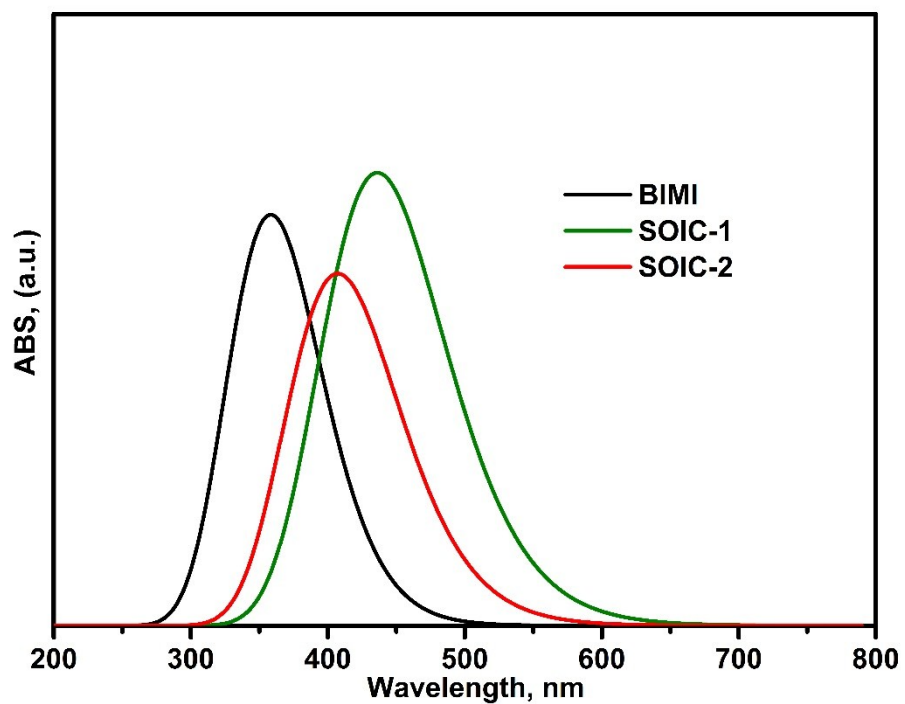


Fig. S9. UV-Vis spectra obtained from TD-DFT calculation.

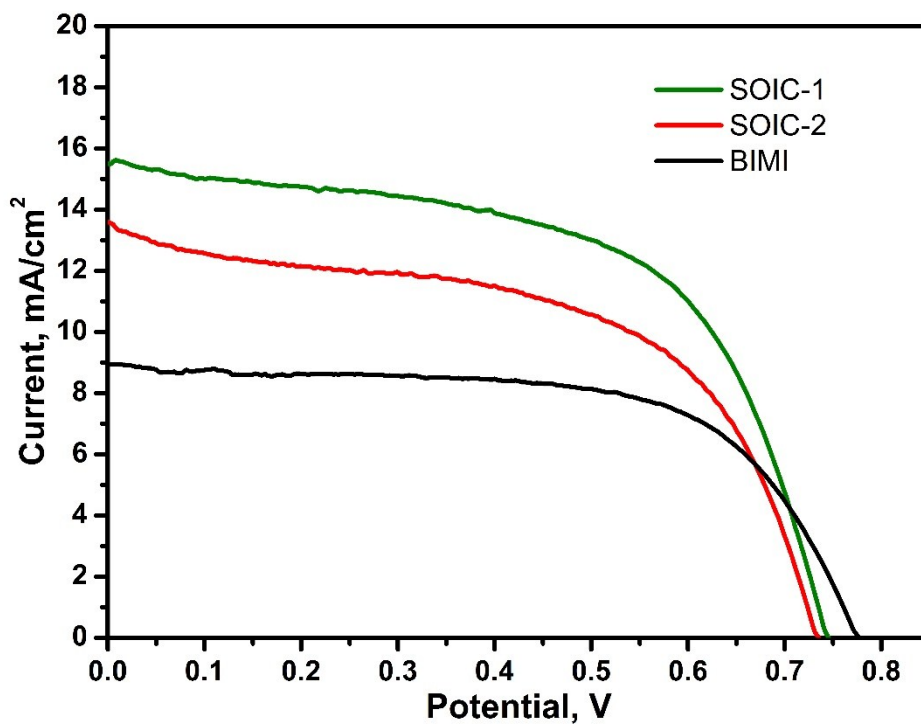


Fig. S10. I-V characteristics of 12 μ m thick TiO₂ photoanode with SOICs and BIMI electrolytes based ss-DSSCs

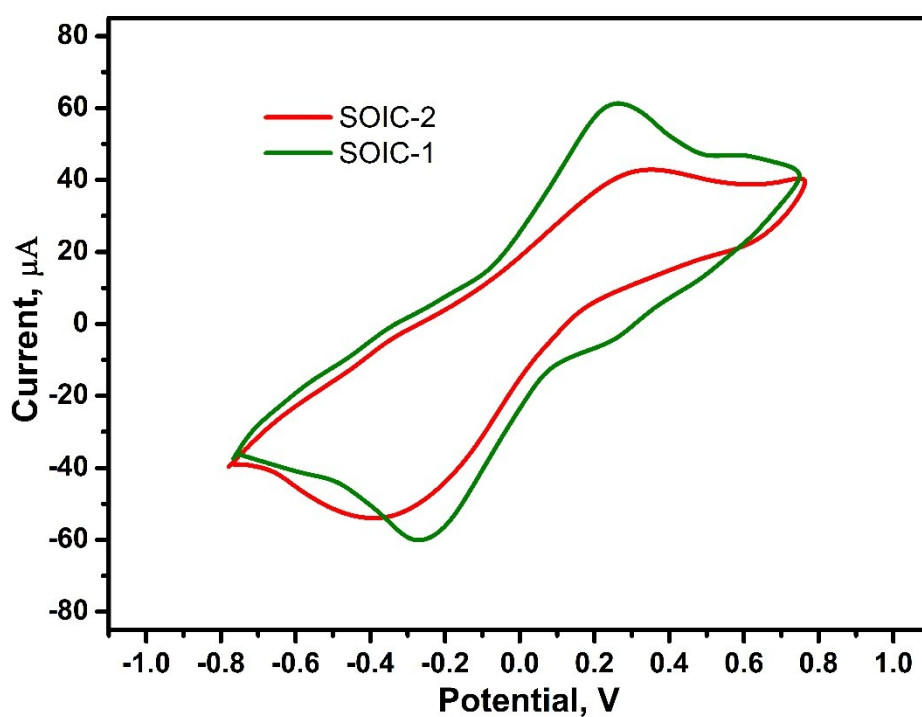


Fig. S11. Solid cyclic voltammetry of SOIC-1 and SOIC-2.

Table S2. Molar extinction coefficient of sensitizer (SK3) and electrolyte (SOICs)

| Sample | λ_{MAX} (nm) | ϵ ($\text{M}^{-1}, \text{cm}^{-1}$) |
|------------|-----------------------------|--|
| SOIC-1 | 377 | 30,076 |
| SOIC-2 | 351 | 29,766 |
| SK-3 | 435 | 17,000 |
| SOIC-1/SK3 | 354,426 | 48,733 |
| SOIC-2/SK3 | 357, 431 | 44,166 |

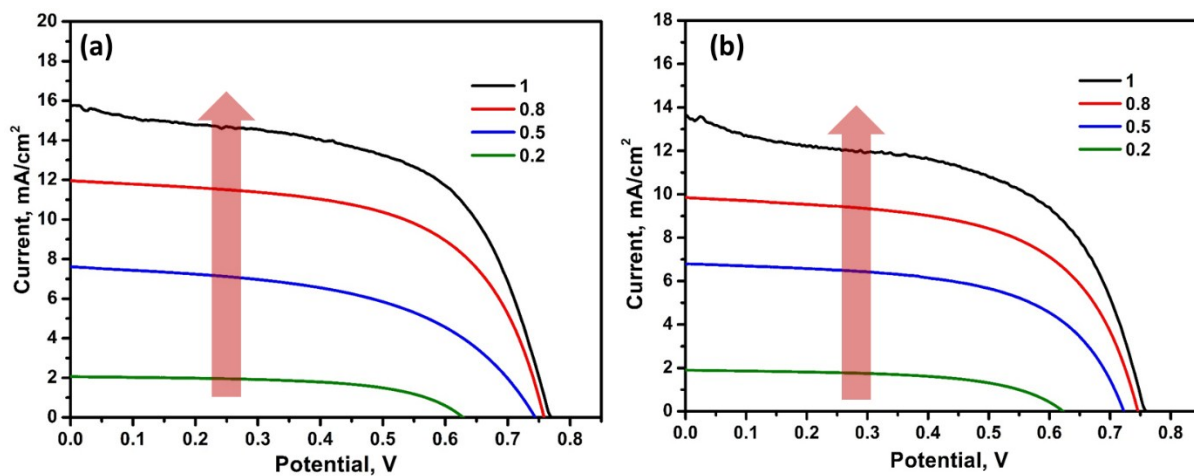


Fig. S12. Influence of illumination on the I - V characteristics of ss-DSSC with SOIC-1 and 2.

Table S3. Photovoltaic parameters of ss-DSSCs at different illumination Intensities

| Devices | Illumination (mW/cm ²) | J_{sc} (mA/cm ²) | V_{oc} (mV) | P_{MAX} | FF (%) | PCE (%) |
|---------|------------------------------------|--------------------------------|---------------|-----------|--------|---------|
| SOIC-1 | 100 | 15.8 | 769 | 7.06 | 58 | 7.10 |
| | 80 | 11.8 | 757 | 5.39 | 60 | 6.74 |
| | 50 | 7.65 | 743 | 2.90 | 51 | 5.79 |
| | 20 | 2.01 | 628 | 0.68 | 53 | 3.34 |
| SOIC-2 | 100 | 13.7 | 759 | 5.69 | 57 | 5.72 |
| | 80 | 9.80 | 745 | 4.32 | 59 | 5.38 |
| | 50 | 6.79 | 722 | 2.72 | 55 | 5.39 |
| | 20 | 1.92 | 625 | 0.63 | 52 | 3.12 |

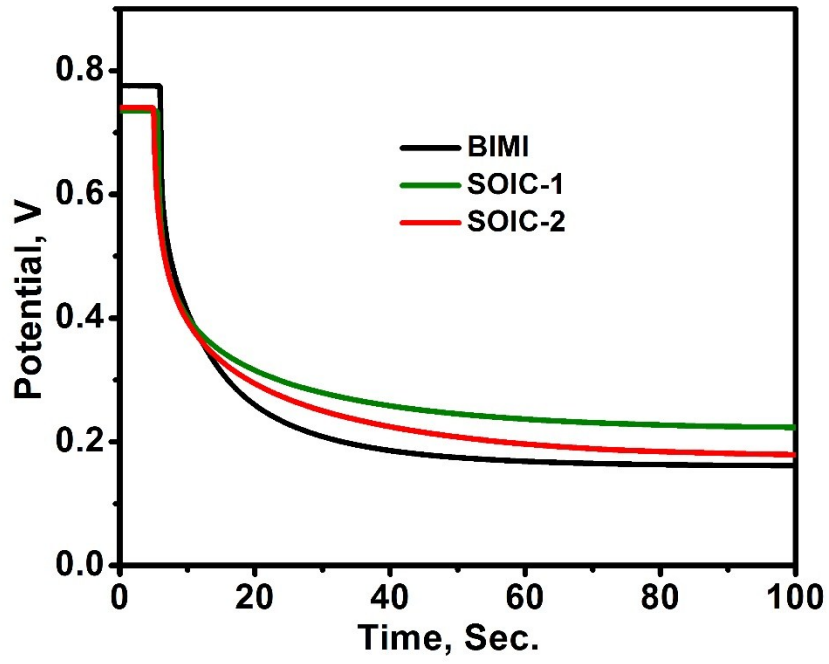


Fig. S13. Open circuit voltage decay curves of ss-DSSCs