Supplementary material for

Phenyl and thienyl functionalized imidazolium iodide for highly efficient quasi-solid state dye-sensitized solar cells

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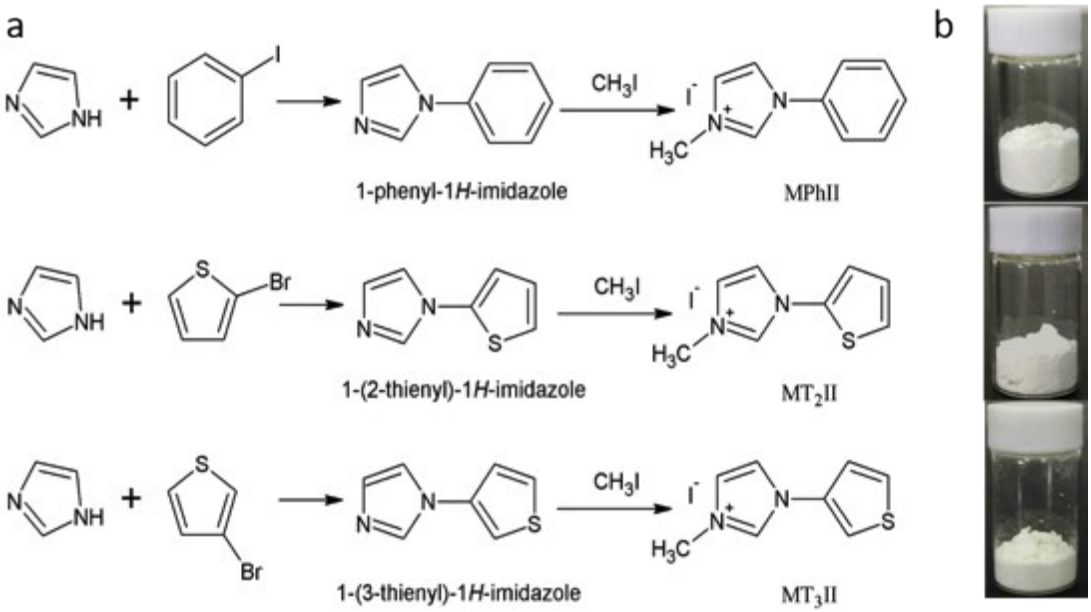

Figure S1. The synthetic route for the ionic conductors and their photographs.

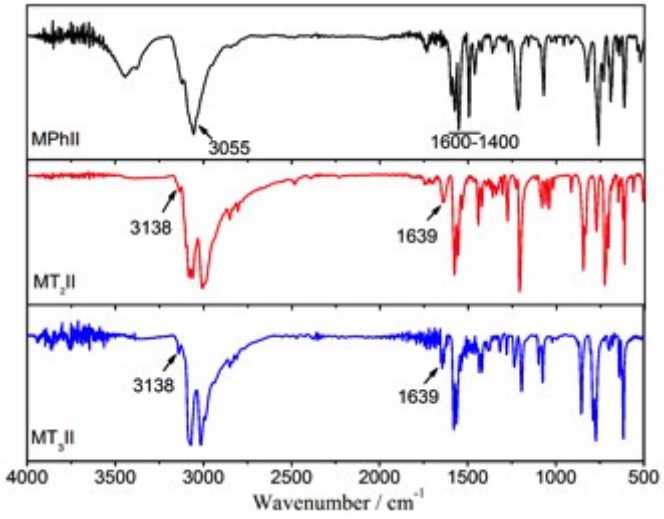

Figure S2. Fourier transform infrared spectra of the three ICs: MPhII, MT_2II and MT_3II.

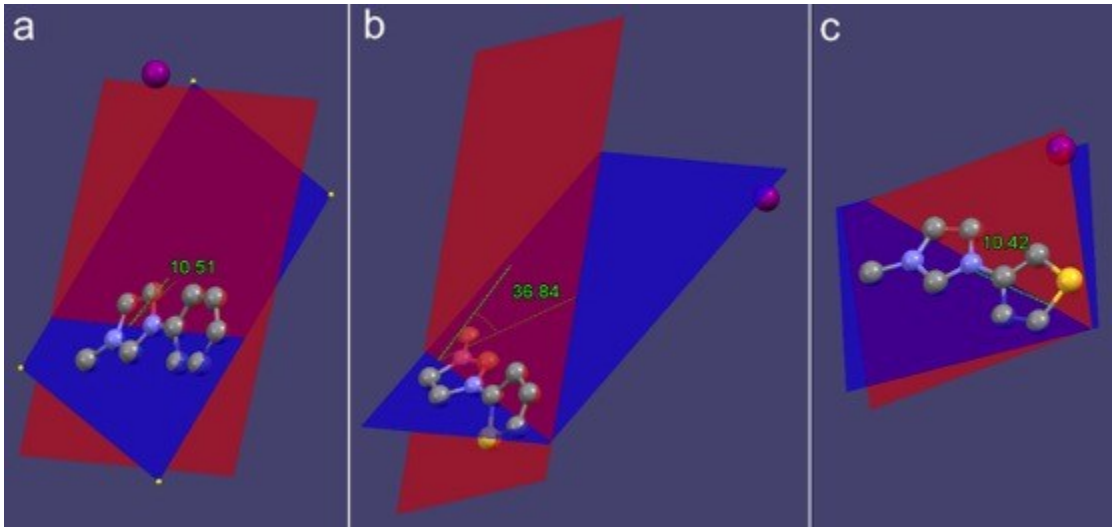

Figure S3. Dihedral angle of imidazolium cation of (a) MPhII, (b) MT_2II, (c) MT_3II.

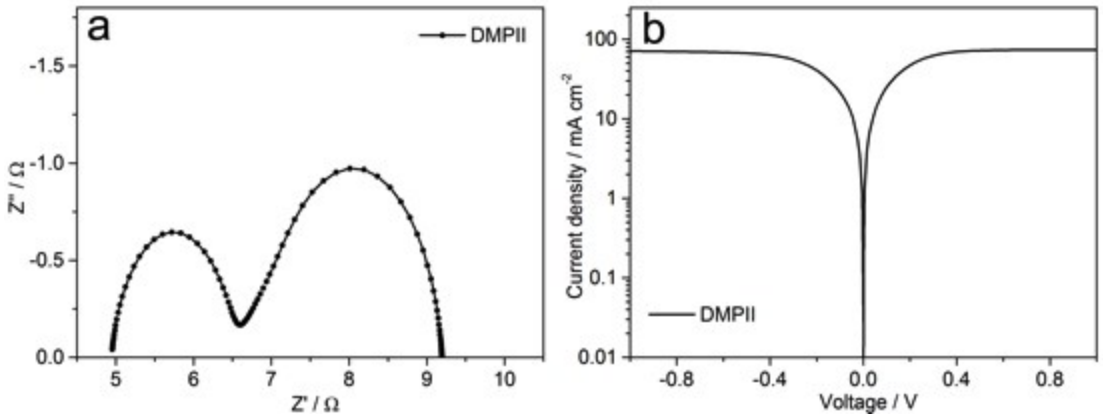

Figure S4. Electrochemical impedance spectroscopy and Tafel polarization curves of the quasi-solid-state electrolyte (QSS-DMPII) containing DMPII, I_2, LiI, TBP (molar ratio, 12/1/2/10) and 4 wt% SiO_2 with 18% solvent of acetonitrile and methanol (1/1, v/v) sandwiched between two platinized FTO substrates.

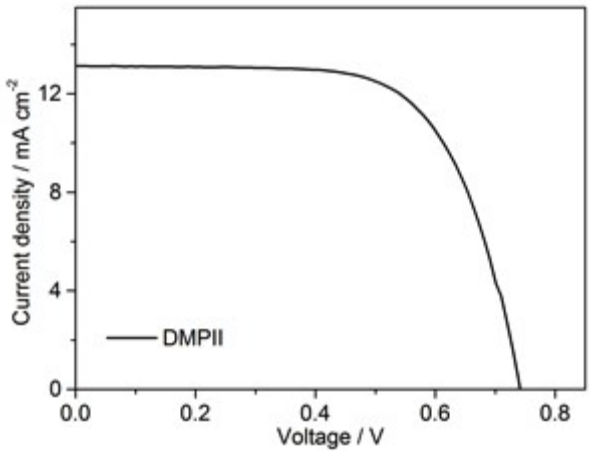

Figure S5. Photocurrent density-voltage characteristics of DSSC based on the QSS-DMPII electrolyte.

Table S1. Crystallographic data (CCDC 1523312) and structural refinement for

MPhII

Ionic conductor	**MPhII**
Empirical formula	C_{10} H_{11} I N_2
Formula weight	286.11
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 8.2438(12) Å, b = 31.628(4) Å, c = 17.204(2) Åα = 90°, β = 93.388(2)°, γ = 90°
Volume	4477.7(11) $Å^3$
Z	16
Calculated density	1.698 Mg/m^3
Absorption coefficient	2.820 mm^{-1}
F(000)	2208
Crystal size	0.12 x 0.10 x 0.06 mm
Theta range for data collection	1.35 to 25.10 °
Limiting indices	-9<=h<=9, -30<=k<=37, -20<=l<=20
Reflections collected	26556
Unique	7940 [R(int) = 0.0458]
Completeness to theta = 25.10	99.7 %
Absorption correction	None
Max. and min. transmission	0.8490 and 0.7284
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7940 / 0 / 473
Goodness-of-fit on F^2	1.108
Final R indices [I>2sigma(I)]	R1 = 0.0699, wR2 = 0.1785
R indices (all data)	R1 = 0.0990, wR2 = 0.1900
Largest diff. peak and hole	0.930 and -1.498 $e.A^{-3}$

Table S2. Crystallographic data (CCDC 1523955) and structural refinement for

MT_2II

Ionic conductor	MT_2II
Empirical formula	$C_8H_9IN_2S$
Formula weight	292.13
Temperature	223(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, Pna21
Unit cell dimensions	a = 18.903(10) Å, b = 6.311(3)Å, c = 17.950(9) Å, $\alpha = 90°$, $\beta = 90°$, $\gamma = 90°$.
Volume	2141.3(19) $Å^3$
Z	8
Density (calculated)	1.812 Mg/m^3
Absorption coefficient	3.138 mm^{-1}
F(000)	1120
Crystal size	0.730 x 0.280 x 0.200 mm^3
Theta range for data collection	2.269 to 27.526°.
Index ranges	-24<=h<=16, -7<=k<=8, -22<=l<=23
Reflections collected	14462
Independent reflections	4864 [R(int) = 0.0349]
Completeness to theta = 25.242°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.647 and 0.328
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4864 / 22 / 238
Goodness-of-fit on F^2	1.122
Final R indices [I>2sigma(I)]	R1 = 0.0419, wR2 = 0.1077
R indices (all data)	R1 = 0.0470, wR2 = 0.1118
Extinction coefficient	0.0025(4)
Largest diff. peak and hole	1.093 and -1.259 e.Å-3

Table S3. Crystallographic data (CCDC 1517957) and structural refinement for

MT_3II

Ionic conductor	MT_3II
Empirical formula	$C_8H_9IN_2S$
Formula weight	292.13
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, Pca21
Unit cell dimensions	a = 19.028(6) Å, b = 7.932(3) Å, c = 13.915(5) Å, α= 90°, β= 90°, γ = 90°
Volume	2100.1(13) $Å^3$
Z	8
Density (calculated)	1.848 Mg/m^3
Absorption coefficient	3.199 mm^{-1}
F(000)	1120
Crystal size	0.470 x 0.430 x 0.290 mm^3
Theta range for data collection	2.141 to 27.511°.
Index ranges	-18<=h<=24, -10<=k<=10, -18<=l<=17
Reflections collected	14077
Independent reflections	4498 [R(int) = 0.0411]
Completeness to theta = 25.242°	99.30%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.430 and 0.192
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4498 / 10 / 224
Goodness-of-fit on F^2	1.091
Final R indices [I>2sigma(I)]	R1 = 0.0300, wR2 = 0.0842
R indices (all data)	R1 = 0.0340, wR2 = 0.0866
Absolute structure parameter	0.03(2)
Extinction coefficient	0.0059(5)
Largest diff. peak and hole	1.093 and -0.633 $e.Å^{-3}$