Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supporting Information

Indoor light harvesting lead-free 2-aminothiazolium bismuth iodide solar cells

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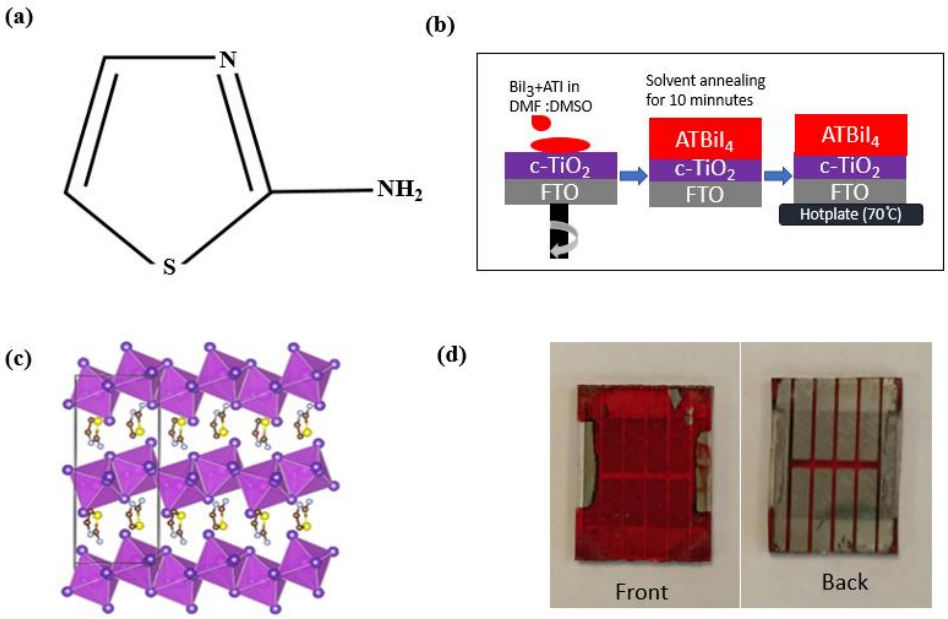

Fig. S1. a) Chemical structure of ATI ligand, b) schematic of the film growth c) crystal structure of $ATBiI_4$ [1] and d) photographs of a fabricated solar cell.

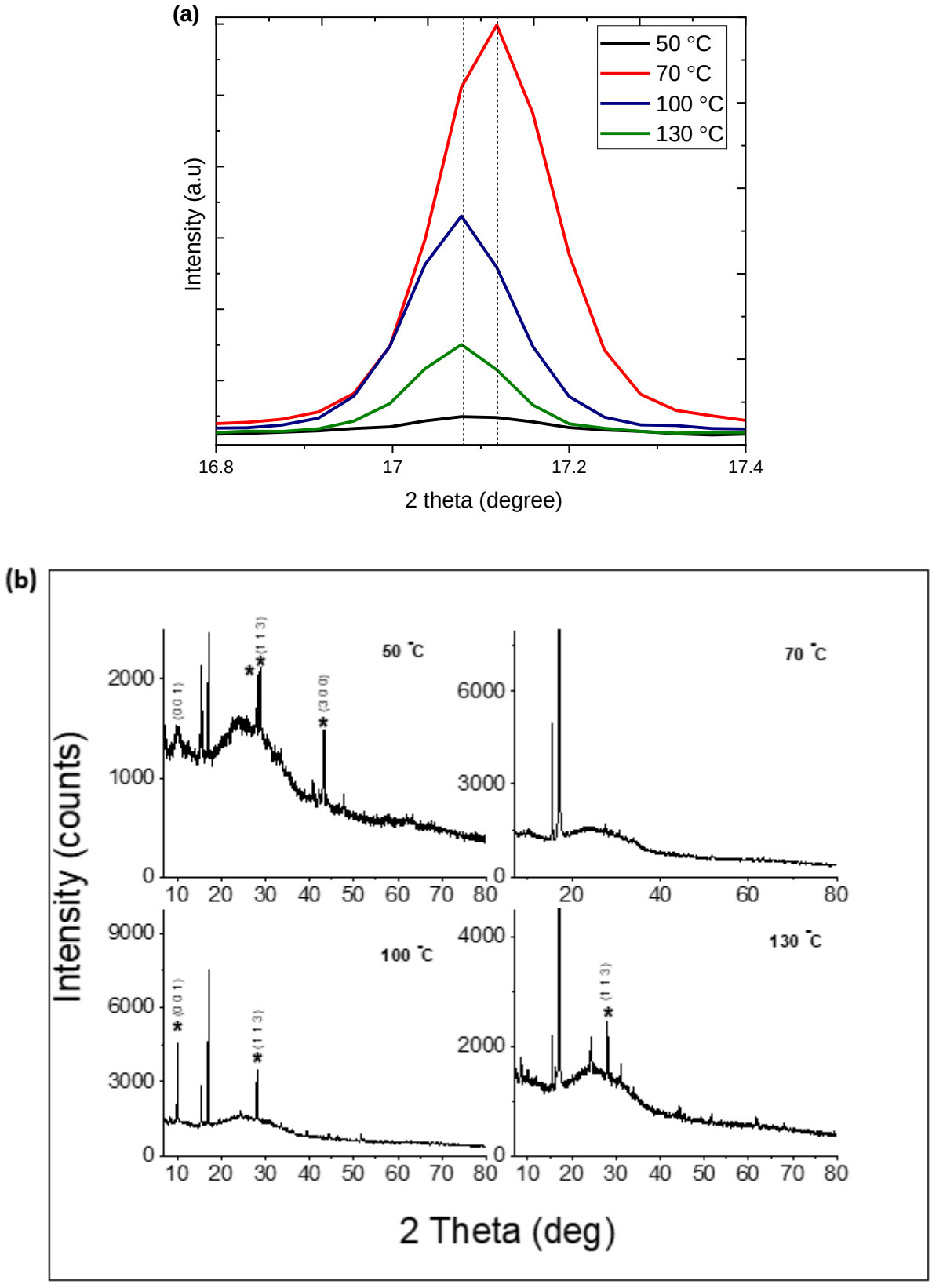

Fig. S2. (a) Enlarged view of the (112) XRD peak and (b) Normalized XRD patterns of the $ATBiI_4$ films annealed at different temperatures with BiI_3 peaks indexed.

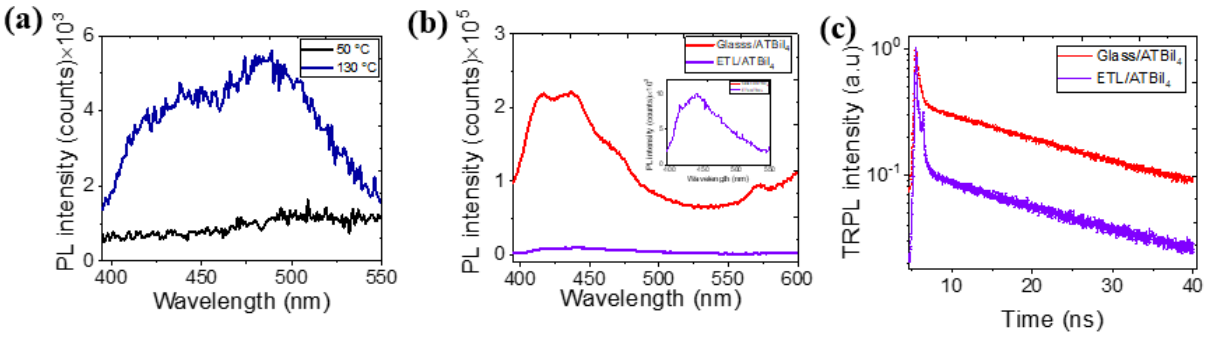

Fig. S3. (a) PL spectra of 50 ℃ and 130 ℃ annealed films, (b) PL spectra of optimal 70 ℃ annealed $ATBiI_4$ films on glass and ETL substrates, and (c) TRPL spectra of the optimal $ATBiI_4$ films on glass and ETL substrates.

Table S1: TRPL decay life time of different temperature annealed $ATBiI_4$ films on glass.

Films	**τ_1 (ns)**	**τ_2 (ns)**	**τ_3 (ns)**	**A_1**	**A_2**	**A_3**	**τ_{avg} (ns)**	**Chi.sq**
50 ℃	0.12	0.12	1.31	120066.27	72023.00	539.93	0.05	269.00
70 ℃	0.45	32.07	-	13138.33	4175.96	-	8.07	19234
100 ℃	0.43	30.59	-	22006.77	3597.85	-	4.66	14702
130 ℃	0.29	17.88	-	31748.38	2048.15	-	1.35	12688.02

*Average decay time is calculated according to the equation: $\tau = (A_1\tau_1 + A_2\tau_2)/(A_1 + A_2)$.

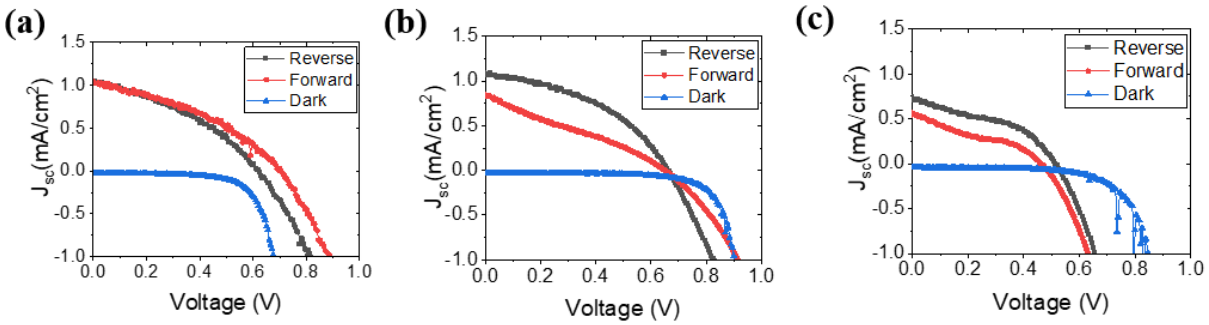

Fig. S4: Reverse and forward scan J-V plot of solar cells based on a) 50 ℃, b) 100 ℃ and c)130 ℃ annealed $ATBiI_4$ films.

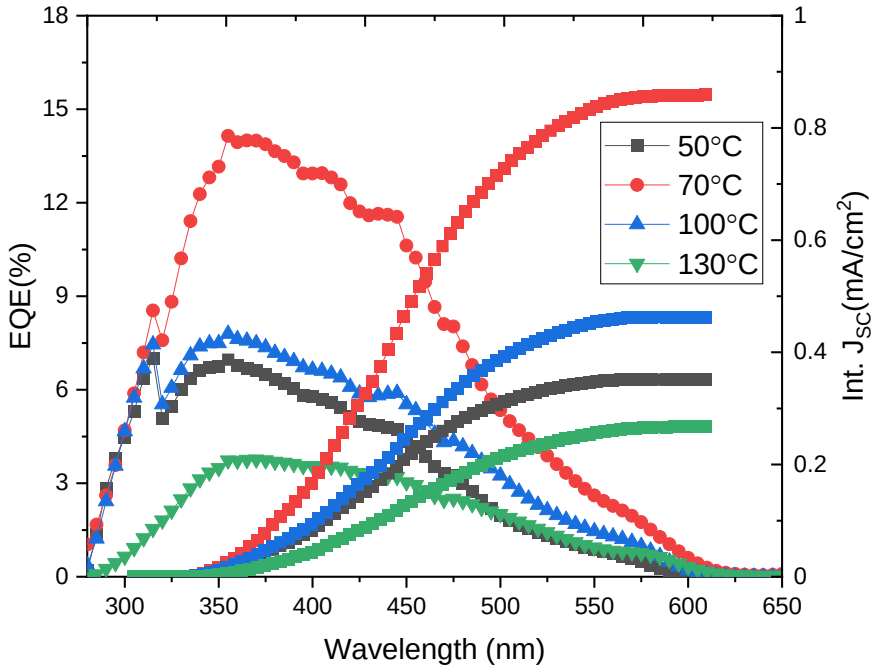

Fig. S5: EQE and integrated J_{sc} spectra of solar cells with $ATBiI_4$ films annealed at 50 ℃, 100 ℃ and 130 ℃.

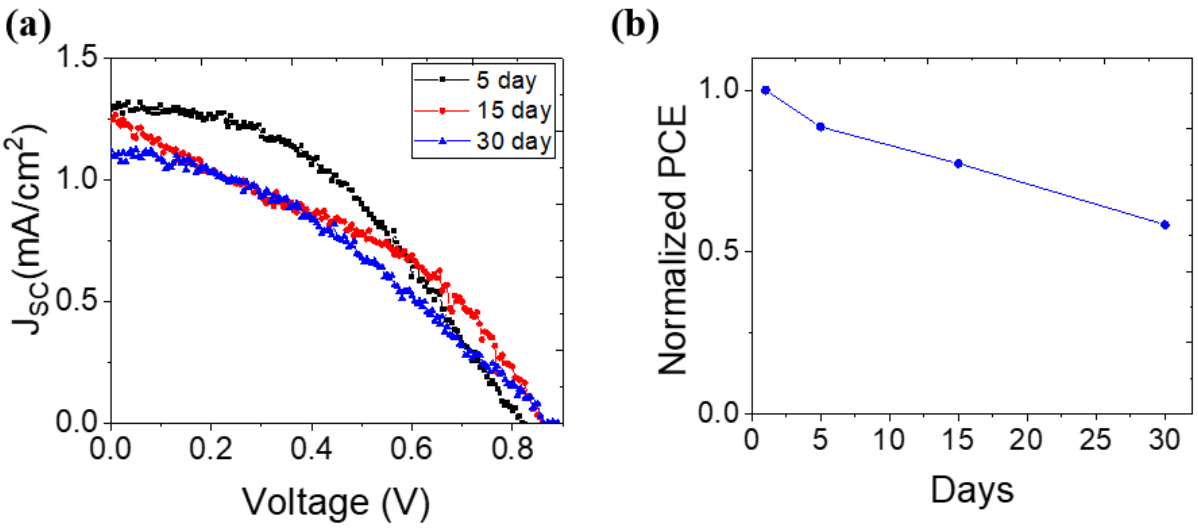

Fig. S6: Aging test of a solar cell with 70℃ annealed $ATBiI_4$ film stored in ambient conditions (Relative humidity: 35-45 %, Temperature: 17-22 ℃). (a) J-V plot of the device tested on varied days and (b) normalized PCE as a function time (in days).

Table S2: Trap densities (n_t) estimated from the ETL and HTL only devices.

Films annealing temperature	n_t **(× 10^{18} cm^{-3})** **(ETL only device)**	n_t **(× 10^{18} cm^{3})** **(HTL only device)**
50 ℃	-	8.93
70 ℃	2.5	3.99
100 ℃	3.7	6.58
130 ℃	-	23.5

Table S3: EIS fitting parameters of $ATBiI_4$ solar cells

Films annealing temperature	$R_s(\Omega)$	R_{ct} (kΩ)
50 ℃	13.83	31.08
70 ℃	3.18	2.42
100 ℃	33.03	15.06
130 ℃	37.60	40.51

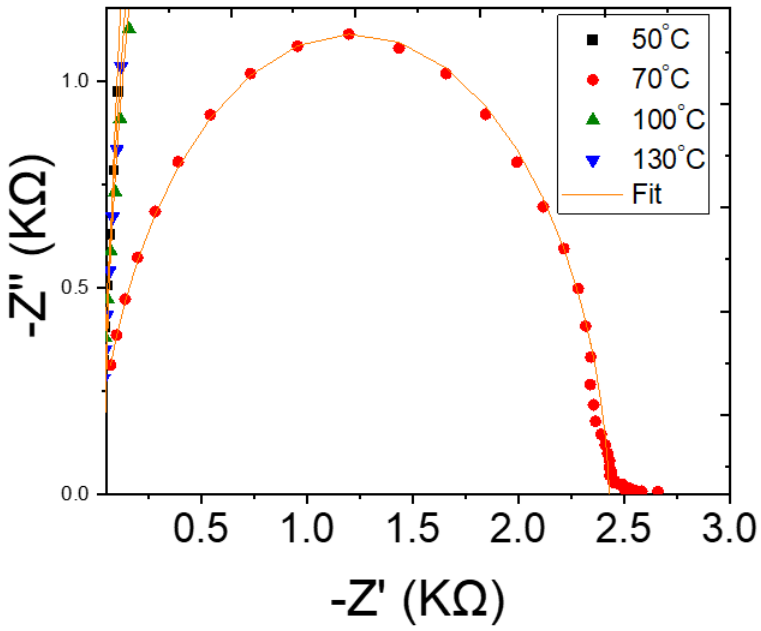

Fig. S7. Magnified view of the Nyquist plot of 70 ℃ annealed $ATBiI_4$ based device with the corresponding fit.

References

1. Li, T., et al., *Extending lead-free hybrid photovoltaic materials to new structures: thiazolium, aminothiazolium and imidazolium iodobismuthates.* Dalton Transactions, 2018. **47**(20): p. 7050-7058.