Supporting Information
Highly efficient heterojunction solar cells enabled by edge-modified tellurene nanoribbons

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TABLE S1: The calculated energy difference ΔE between HE-ZTNR and TE-ZTNR (meV per atom).

Width of ZTNR	ΔE
4	7.11
5	7.19
6	6.70
7	4.56
8	5.32
9	5.80
10	3.02
11	3.78

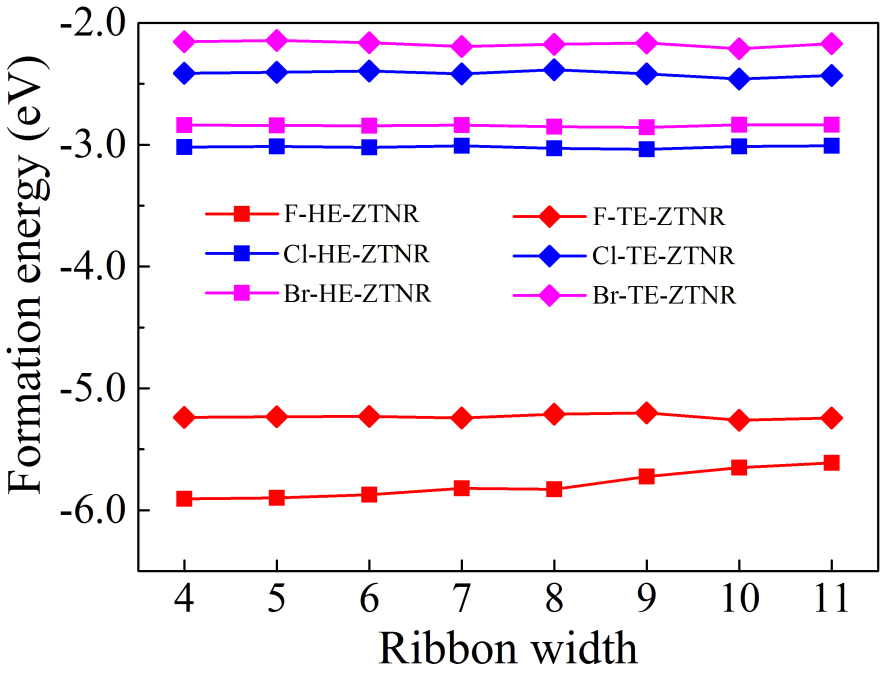

FIG. S1: The calculated formation energy of edge-modified ZTNRs as a function of the ribbon width.

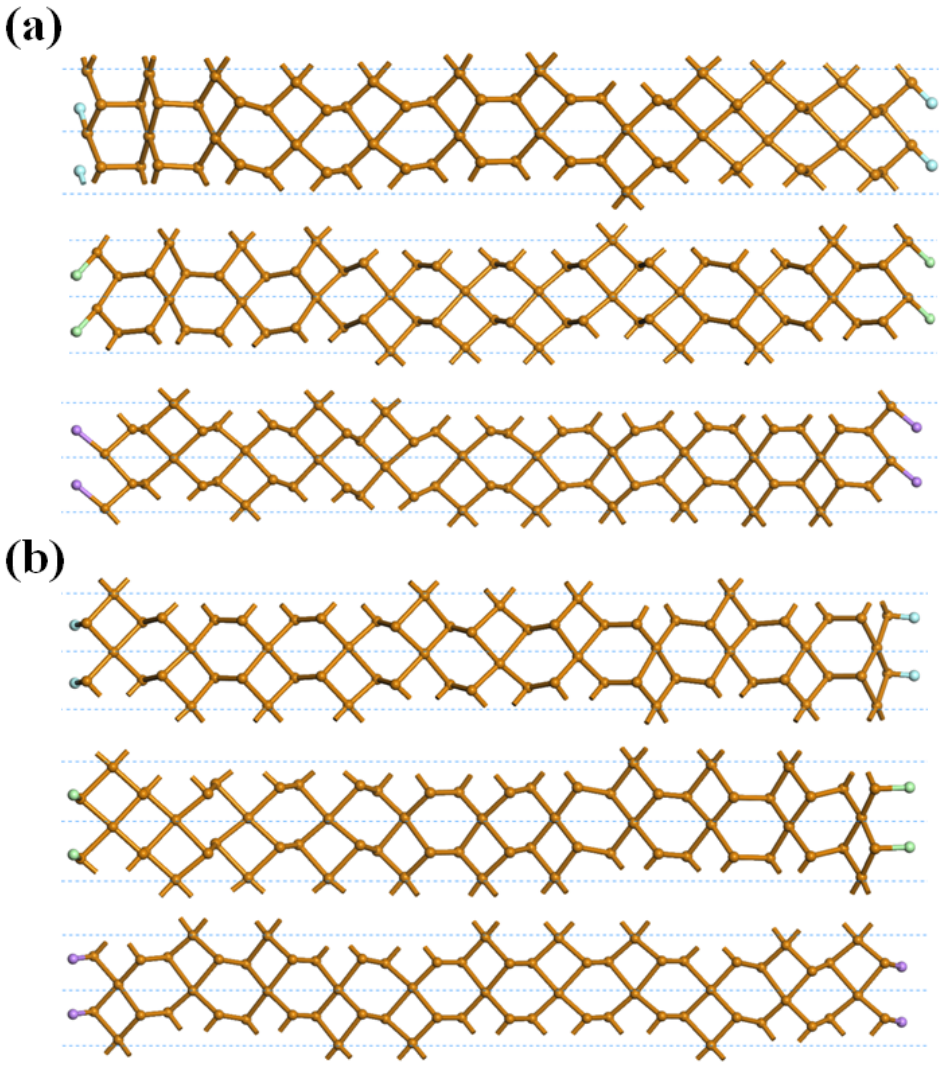

FIG. S2: AIMD simulations of X-ZTNR-11 (X = H, F, Cl and Br). Atomic structures of (a) X-HE-ZTNR-11 and (b) X-TE-ZTNR-11 after AIMD fluctuations for 10.0 ps at T = 300 K. The orange, white, cyan, light green and purple balls denote tellurium, hydrogen, fluorine, chlorine and bromine atoms, respectively.

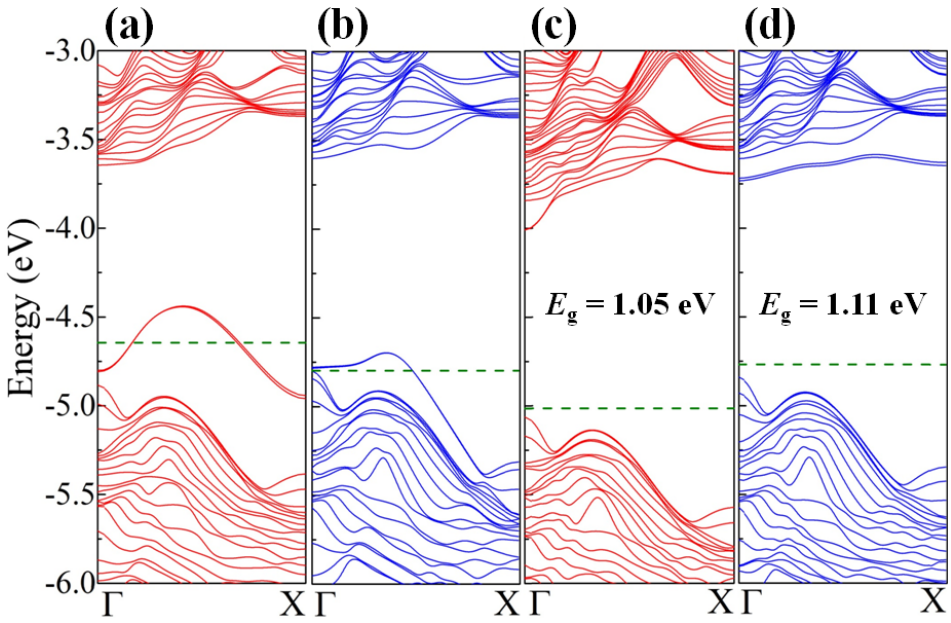

FIG. S3: The band structures of (a) HE-ZTNR-10, (b) TE-ZTNR-10, (c) Br-HE-ZTNR-10 and (d) Br-TE-ZTNR-10 calculated by PBE functional. HE-ZTNR-10 and TE-ZTNR-10 show like metal. The band gaps E_g of Br-HE-ZTNR-10 and Br-TE-ZTNR-10 are marked in each diagram. The green dash lines denote fermi energy level. The vacuum energy level is set to zero.

TABLE S2: The calculated binding energy E_b (meV per atom) and equilibrium distance D (Å) of ZTNRs heterobilayers and bilayer tellurene for comparison.

Heterobilayer	E_b	D
F/Cl-HE-ZTNRs-11	-78.2	2.38
F/Br-HE-ZTNRs-11	-80.1	2.32
Cl/Br-HE-ZTNRs-11	-74.6	2.40
F/Cl-TE-ZTNRs-11	-74.4	2.41
F/Br-TE-ZTNRs-11	-75.3	2.39
Cl/Br-TE-ZTNRs-11	-75.2	2.38
Bilayer tellurene	-75.0	2.43

TABLE S3: Power conversion efficiency (PCE) of our proposed heterojunction solar cells based on ZTNRs with width varying from 9 to 10. Relative properties are also listed, including band gap of donor semiconductor E_{d} (eV) and conduction band offset ΔE_{c} (eV).

ZTNRs Heterobilayer	E_{d}	ΔE_{c}	PCE (%)
F/Cl-HE-ZTNRs-9	1.49	0.264	17.9
F/Br-HE-ZTNRs-9	1.49	0.197	19.1
Cl/Br-HE-ZTNRs-9	1.40	0.067	21.6
F/Cl-HE-ZTNRs-10	1.48	0.235	18.5
F/Br-HE-ZTNRs-10	1.48	0.157	19.8
Cl/Br-HE-ZTNRs-10	1.39	0.077	21.4
F/Cl-TE-ZTNRs-9	1.47	0.056	21.6
F/Br-TE-ZTNRs-9	1.47	0.093	20.8
Cl/Br-TE-ZTNRs-9	1.47	0.038	22.0
F/Cl-TE-ZTNRs-10	1.44	0.066	21.5
F/Br-TE-ZTNRs-10	1.44	0.880	21.1
Cl/Br-TE-ZTNRs-10	1.44	0.021	22.5