

Supplementary Information

Side-chain Engineering of Conjugated Molecules for N-type Organic Thermoelectrics

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Table S1 Summary of thermoelectric parameters for n-type materials, including the maximum power factor (PF_{max}) and its corresponding electrical conductivity (σ) and Seebeck coefficient (S) at PF_{max} . Data were sourced directly from the text of the literatures or extracted from figures within the cited works.

Material	Dopant	Year	σ (S/cm)	S (μ V/K)	PF_{max} (μ W/mK ²)	DOI
CNg4T2-CNT2	N-DMBI	2024	13.2	-94	10.84	10.1039/D3FD00135K
CNg4T2-2FT	N-DMBI	2024	0.21	-149	0.46	10.1039/D3FD00135K
ThDPP-CNBTz	N-DMBI	2024	50.6	-145	105.10	10.1002/anie.202402642
PTTz1	N-DMBI	2024	10.5	-114	12.50	10.1021/acsami.4c08553
PTTz2	N-DMBI	2024	50.3	-69	23.80	10.1021/acsami.4c08553
f-BTI2g-SVSCN	TAM	2024	43.91	-93	37.90	10.1002/anie.202408537
f-BTI2g-SVSCN	N-DMBI	2024	47.9	-74	26.10	10.1002/anie.202408537
f-BTI2g-SVSCN	JLBI	2024	84.9	-83	57.90	10.1002/anie.202408537
f-BSeI2g-SVSCN	TAM	2024	187.3	-63	73.40	10.1002/anie.202408537
f-BSeI2g-SVSCN	N-DMBI	2024	152.5	-61	56.00	10.1002/anie.202408537
f-BSeI2g-SVSCN	JLBI	2024	101.2	-106	114.10	10.1002/anie.202408537
n-PT5	PEI	2024	31.3	-109	36.90	10.1002/adv.202401952
n-PT5	N-DMBI	2024	36.2	-69	18.20	10.1002/adv.202401952
PBDP-2CN	TDAE	2024	0.065	-384	1.3	10.1021/acs.chemmater.4c01894
pDSe	N-DMBI	2024	5.9	-218	27.80	10.1002/anie.202409018
pDFSe	N-DMBI	2024	62.6	-146	133.10	10.1002/anie.202409018
PBFDOTh-T	N-DMBI	2024	4.72	-127	7.70	10.1039/D4TC02516D
PBFDOTh-Se	N-DMBI	2024	8.6	-162	22.70	10.1039/D4TC02516D
DPP-BFDO-Th	N-DMBI	2024	0.0703	-349	0.86	10.1002/anie.202402375
DPP-BFDO	N-DMBI	2024	35.27	-84	24.53	10.1002/anie.202402375
P-B3O	N-DMBI	2024	0.026	-239	0.15	10.1021/acsmaterialslett.4c00068
P-6O	N-DMBI	2024	3.3	-115	4.30	10.1021/acsmaterialslett.4c00068
P-3O	N-DMBI	2024	9	-130	15.30	10.1021/acsmaterialslett.4c00068
P(DPP-CNPz)	N-DMBI	2024	25.3	-132	41.40	10.1002/anie.202319658
P(DPP-DCNPz)	N-DMBI	2024	33.93	-95	30.40	10.1002/anie.202319658
P-3O	N-DMBI	2024	5.7	-211	25.30	10.1039/D3TA07188J

f-BSeI2TEG-T	N-DMBI	2023	7.1	-112	8.80	10.1002/adfm.202213911
f-BSeI2TEG-FT	N-DMBI	2023	87.9	-89	70.10	10.1002/adfm.202213911
TBDOPV-T-518	N-DMBI	2023	68.95	-181	230.00	10.1126/sciadv.adf3495
n-PT1	TDAE	2023	61.2	-160	141.70	10.1002/anie.202216049
P(NDI2OD-T2)	IStBI	2023	0.00257	-128	0.00	10.1002/admi.202202416
PDPIN	N-DMBI	2023	19.1	-100	19.00	10.1002/anie.202219313
PDPIN	PSpF	2023	78.1	-145	163.00	10.1002/anie.202219313
PC61BM	P2-t-Bu	2023	2.64	-202	11.02	10.1002/adma.202300084
PC61BM	P4-t-Bu	2023	1.08498	-268	7.78	10.1002/adma.202300084
PDCNBT-DPP	N-DMBI	2023	3.72	-146	7.96	10.1038/s41428-022-00717-w
PDCNBS-e-DPP	N-DMBI	2023	8.83	-102	9.22	10.1038/s41428-022-00717-w
PTQDPP-2FT	N-DMBI	2023	0.00212	-796	1.34	10.1002/adfm.202300809
PTQDPP-T	N-DMBI	2023	0.0093	-944	0.83	10.1002/adfm.202300809
n-PT3	N-DMBI	2023	100.8	-106	110.00	10.1002/adma.202309679
n-PT4	N-DMBI	2023	123.3	-90	100.60	10.1002/adma.202309679
n-PT4	DMImC	2023	50.15239	-177	157.30	10.1002/adma.202309679
BTCNOg-FT	N-DMBI	2023	0.51	-172	1.50	10.1021/acs.macromol.2c02564
BTOgCN-FT	N-DMBI	2023	0.83	-181	2.77	10.1021/acs.macromol.2c02564
NDI-T1/SWCNT	N-DMBI	2023	730.5	-58	240.60	10.1002/sml.202306166
PTz-5-DPP	N-DMBI	2023	8.18	-353	102.00	10.1002/anie.202219262
PCNI2-V	N-DMBI	2023	1.3	-44	0.22	10.1002/adma.202210847
PCNI2-T	N-DMBI	2023	11.3	-69	5.29	10.1002/adma.202210847
PCNI2-BTI	N-DMBI	2023	81.51229	-115	107.80	10.1002/adma.202210847
PO8	N-DMBI	2023	12.1047	-110	14.70	10.1002/advs.202302629
PO12	N-DMBI	2023	35.84347	-162	94.30	10.1002/advs.202302629
PO16	N-DMBI	2023	14.29253	-156	34.76	10.1002/advs.202302629
C12NR	N-DMBI	2022	0.97	-79	0.60	10.1002/advs.202204872
PFCITVT	PSpF	2022	2.2	-550	67.00	10.1002/adma.202201062
PBFDO	-	2022	2000	-21	90.00	10.1038/s41586-022-05295-8
PDTzTI-TEG	N-DMBI	2022	34	-68	15.70	10.1002/ange.202214192
PIQ-A	N-DMBI	2022	0.0072	-1062	0.81	10.1021/acs.macromol.2c01029
PIQ-O	N-DMBI	2022	0.27977	-389	4.24	10.1021/acs.macromol.2c01029
P-75	N-DMBI	2021	12	-105	13.20	10.1002/anie.202113078
PCIBD	TP-DMBI	2021	1	-560	32.00	10.1002/anie.202110505
PFCITVT	N-DMBI	2021	3.62069	-250	22.70	10.1002/adfm.202005901
PCICITVT	N-DMBI	2021	0.08838	-927	7.60	10.1002/adfm.202005901
PFCITVT	CoCp2	2021	0.67798	-763	39.50	10.1002/adfm.202005901
PCICITVT	CoCp2	2021	0.11829	-822	8.00	10.1002/adfm.202005901
N-N	N-DMBI	2021	0.50845	-251	3.20	10.1021/jacs.0c10365
N-A	N-DMBI	2021	0.26	-241	1.60	10.1021/jacs.0c10365
A-A	N-DMBI	2021	0.018	-368	0.25	10.1021/jacs.0c10365
PBN-19	TDAE	2021	7.8	-179	24.80	10.1002/anie.202105127
PNDICITVT	NDI-TBAF	2021	0.2	-1854	67.00	10.1002/adfm.202010567
PNDI2TEG-T2DEG	N-DMBI	2021	0.05	-219	0.24	10.1021/acs.macromol.1c00317
BBL	BV ⁺	2021	1.23	-208	5.37	10.1039/D1TA01645H
f-BTI2TEG-FT+PBTI	N-DMBI	2021	104	-80	65.70	10.1038/s41586-021-03942-0
PCNI-BTI	N-DMBI	2021	14.4	-83	10.00	10.1021/jacs.0c11608
PNDI2HexEG-2Tz	N-DMBI	2021	3.3	-115	4.30	10.1002/adma.202006694
PNDI2C8TEG-2Tz	N-DMBI	2021	1.7	-326	18.00	10.1002/adma.202006694

TBDPPV	N-DMBI	2020	58.2	-114	76.00	10.1002/adma.202005946
TBDOPV-T	N-DMBI	2020	57.3	-136	106.00	10.1002/adma.202005946
TBDOPV-2T	N-DMBI	2020	0.6	-330	6.00	10.1002/adma.202005946
PI-BN	N-DMBI	2020	9.70E-04	-454	0.02	10.1021/acsami.9b21527
BBL	PEI	2020	5.3	-144	11.00	10.1038/s41467-021-22528-y
FBDPPV	TAM	2020	18	-168	51.00	10.1038/s41467-020-17063-1
PTEG-2	N-DMBI	2020	8.3	-222	41.00	10.1038/s41467-020-19537-8
UFBDDPPV	TAM	2020	22	-198	80.00	10.1021/jacs.0c05699
UFBDDPPV	N-DMBI	2020	16	-94	11.60	10.1021/jacs.0c05699
pNB	N-DMBI	2020	0.011	-500	0.30	10.1002/adma.202002060
pNB-Tz	N-DMBI	2020	0.87	-350	9.90	10.1002/adma.202002060
pNB-TzDP	N-DMBI	2020	11.6	-214	53.40	10.1002/adma.202002060
BBL	N-DMBI	2020	1.1	-112	1.50	10.1021/acsami.0c16254
PDTzTI	TDAE	2019	4.6	-129	7.60	10.1021/acsenergylett.9b00977
LPPV-1	N-DMBI	2019	0.66	-172	1.96	10.1002/anie.201905835
LPPV-2	N-DMBI	2019	0.055	-214	0.25	10.1002/anie.201905835
P(TDPP-CT2)	N-DMBI	2019	0.25	-607	9.30	10.1021/jacs.9b10107
P(PzDPP-CT2)	N-DMBI	2019	3.99	-379	57.30	10.1021/jacs.9b10107
PPA	N-DMBI	2018	0.10202	-193	0.38	10.1016/j.nanoen.2018.07.056
PDEG-1	N-DMBI	2018	1.06206	-294	9.18	10.1016/j.nanoen.2018.07.056
PTeEG-1	N-DMBI	2018	2.27002	-319	23.10	10.1016/j.nanoen.2018.07.056
PPEG-1	N-DMBI	2018	1.37939	-266	9.76	10.1016/j.nanoen.2018.07.056
PDPF	N-DMBI	2018	0.84	-235	4.65	10.1002/adma.201802850
P(NDI2OD-Tz2)	TDAE	2018	0.07	-462	1.50	10.1002/adma.201801898
2Strans-PNDIT2	N-DPBI	2018	0.006	-90	0.05	10.1021/acsaem.8b00777
TEG-N2200	N-DMBI	2018	0.17	-153	0.40	10.1002/adma.201704630
p(gNDI-gT2)	N-DMBI	2018	0.11	-190	0.40	10.1021/acsenergylett.7b01146
PNDI2TEG-2Tz	N-DMBI	2018	1.8	-159	4.50	10.1002/adma.201804290
PTEG-1	N-DMBI	2017	2.05	-285	16.70	10.1002/adma.201701641
PNDTI-BBT-DP	N-DMBI	2017	5	-169	14.00	10.1021/acs.macromol.6b02313
A-DCV-DPPTT	N-DMBI	2017	3.1	-568	95.00	10.1021/jacs.7b05344
Q-DCM-DPPTT	N-DMBI	2017	0.11	-383	1.70	10.1021/jacs.7b05344
CIBDPPV	TBAF	2017	0.62	-99	0.63	10.1002/adma.201606928
BBL	TDAE	2016	0.93	-68	0.43	10.1002/adma.201603731
P(PymPh)	NaNap	2016	18	-16	0.49	10.1039/C6CP04572C
FBDPPV	N-DMBI	2016	6.23	-210	25.50	10.1021/acsami.6b06899
BDPPV	N-DMBI	2015	0.26	-310	2.50	10.1021/jacs.5b00945
CIBDPPV	N-DMBI	2015	4	-210	17.00	10.1021/jacs.5b00945
FBDPPV	N-DMBI	2015	7	-200	28.00	10.1021/jacs.5b00945
