

Supplementary Information

The cyclic voltammetry measurement

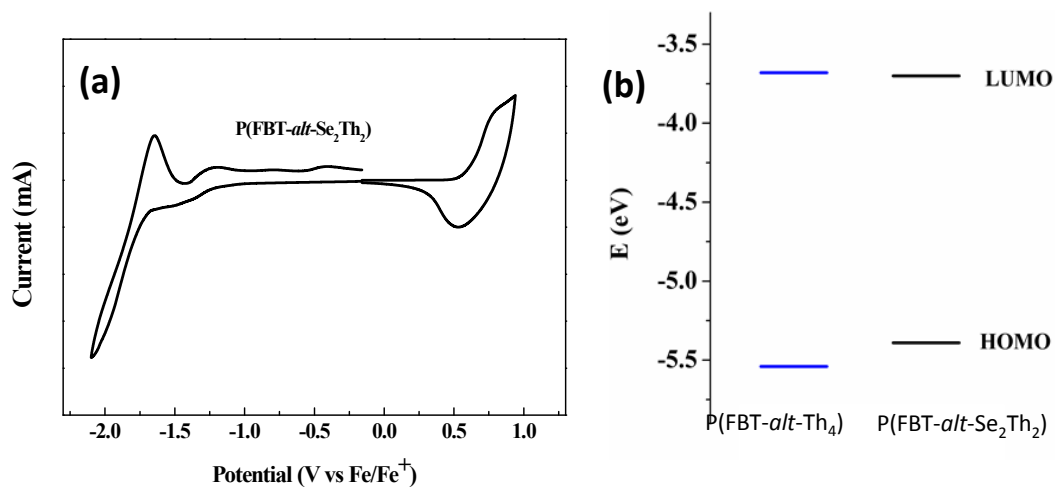


Figure S1. (a) Cyclic voltammogram of **P(FBT-*alt*-Se₂Th₂)** and (b) illustration of the E_{HOMOS} and E_{LUMOS} of the **P(FBT-*alt*-CP₄)** copolymers.

The TGA measurement

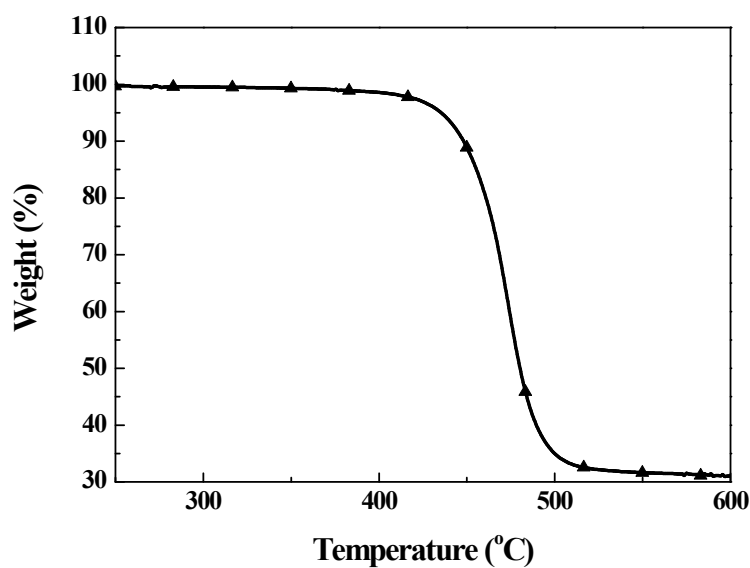


Figure S2. Thermogravimetric analysis of **P(FBT-*alt*-Se₂Th₂)**.

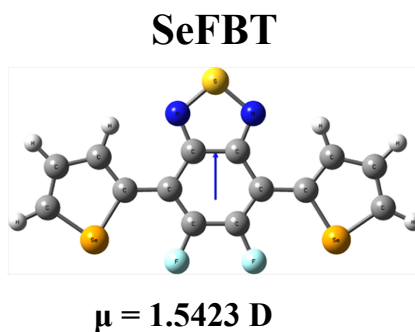
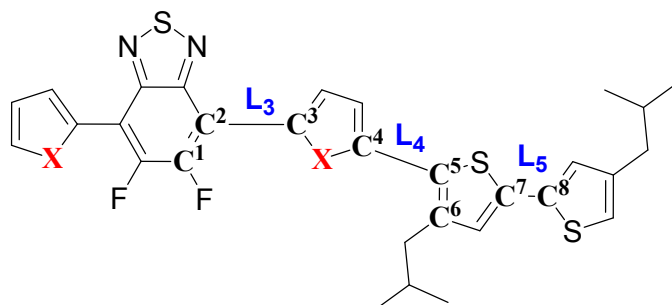


Figure S3. Illustration of the dipole moment of the **SeFBT** unit. Blue arrow indicates the direction of the dipole moment. The length of the blue arrow is decided by the strength of the dipole moment. The unit of the dipole moment is given in Debye.

Table S1. Calculated interannular bond lengths of the repeat units of **P(FBT-*alt*-Se₂Th₂)** and **P(FBT-*alt*-Th₄)**^a

	X	L ₃ (Å)	L ₄ (Å)	L ₅ (Å)
P(FBT-<i>alt</i>-Th₄)	S	1.46	1.46	1.45
P(FBT-<i>alt</i>-Se₂Th₂)	Se	1.46	1.46	1.45

a. Illustration and definition of L₃, L₄, and L₅



L₃:bond length of C₂-C₃,L₄:bondlength of C₄-C₅,L₅:bondlength of C₇-C₈.

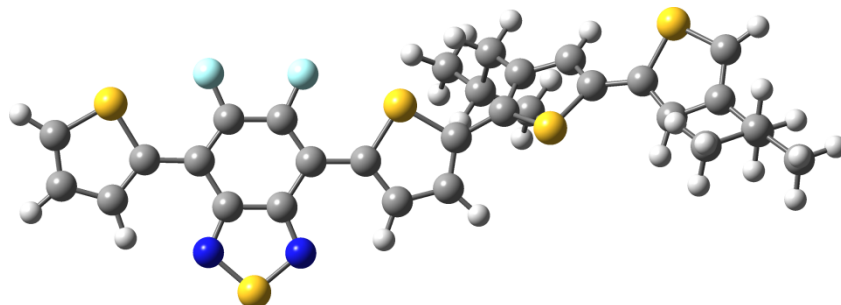
Computational details

Quantum-chemical calculations were performed with the Gaussian09 suite² employing the WB97XD density functional in combination with the 6-311G(d,p) basis set. Geometry optimizations were performed with tight SCF and convergence criteria and an ultrafine integration grid by applying the GEDIIS optimization algorithm. The minimum nature of each stationary point was confirmed by a frequency analysis.

Cartesian coordinates (Å) and energies (Hartree) of the Gaussian

WB97XD/6-311G(d,p) optimized structures:

FBT-Th₄

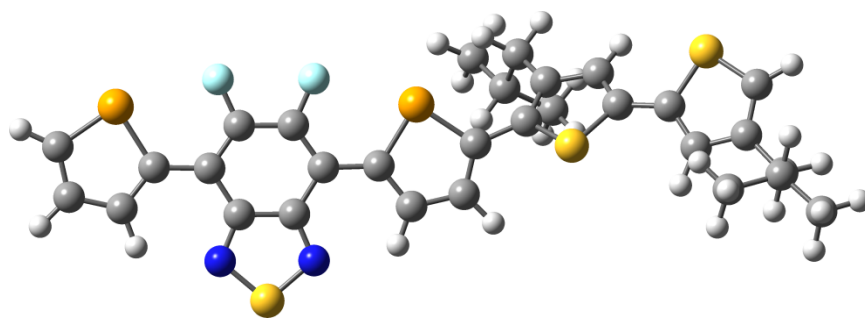


E=−3458.85647406 ($N_{\text{img}} = 0$)

C	−5.157074303692	−0.428876562267	−0.998433878433
C	−3.758964223732	−0.440039062217	−0.726711383748
C	−3.130831227866	0.376167568951	0.170044035725
C	−4.035660083056	1.282459850622	0.835595378265
C	−5.457867412949	1.294783747226	0.557606838291
C	−6.061459542962	0.401830603608	−0.401867532547
N	−6.108730976687	2.203921893773	1.270828397709
N	−3.685877218056	2.182037515189	1.744992881502
S	−5.026421951194	2.967328873136	2.202315790724
F	−3.069283112630	−1.338033737147	−1.433357830332
F	−5.545358476913	−1.318311745720	−1.914228991064
C	−1.694629911803	0.345890353083	0.434445769895
C	−0.995226270761	1.095001229245	1.349845056664
S	−0.603309967685	−0.710309430313	−0.428589313670
C	0.388340590026	0.814351346711	1.369511233236
H	−1.471904881809	1.816958258952	1.993102090817
C	0.759683963202	−0.150652387100	0.472679901903
H	1.090461105894	1.291228153540	2.040456076222
C	−7.494016461232	0.395174546781	−0.694064950462
C	−8.480404514203	1.108356278634	−0.056000951349
S	−8.188207377889	−0.566370242120	−1.976491558939
C	−9.772506049734	0.885400487954	−0.589813897616
H	−8.273458166638	1.774383359611	0.766154684202
C	−9.763261719087	0.008589906449	−1.630939229766
H	−10.668515609412	1.359086339900	−0.213011123128
H	−10.599417805075	−0.340178437682	−2.218147256295
C	2.100480982700	−0.670772964321	0.226506694201
C	2.534524400258	−1.971402698404	0.146019006959
S	3.410849241045	0.450179368174	0.025281623716

C	3.940291244491	-2.045835313725	-0.053196120628
C	4.563201571091	-0.831018323506	-0.126617764098
H	4.478078094385	-2.984702410996	-0.104545810155
C	5.976215003014	-0.543507194766	-0.316822692821
C	6.701643240713	0.514745321402	0.154924474260
S	6.982445082292	-1.603411268322	-1.250069213907
C	8.077085308882	0.484260154509	-0.218675036078
C	8.364330190493	-0.616110319271	-0.971441771110
H	9.321531785025	-0.902496151030	-1.382241070734
C	1.669557710562	-3.186537893899	0.354204894106
H	0.830623922274	-3.180608446991	-0.347353057548
H	2.258410068674	-4.080214085377	0.118388969136
C	1.123723170644	-3.316701252685	1.788167983300
H	0.543613207429	-2.412583114492	2.006652662931
C	2.256701626684	-3.411677692923	2.808633106531
H	2.909328172843	-2.536060959870	2.764157074339
H	1.860343368843	-3.486859967180	3.824818512483
H	2.871384321332	-4.299924386073	2.622444921256
C	0.185037279285	-4.517658349895	1.884673205538
H	0.719105041365	-5.447561417525	1.659379947054
H	-0.233112741597	-4.609358961277	2.890743685168
H	-0.646936705179	-4.427922197715	1.180243855519
H	6.272348229475	1.291055458106	0.776641919725
C	9.074841670689	1.550826765068	0.138014918955
H	10.048511369547	1.087879303895	0.327627614332
H	8.771336216666	2.033200979136	1.074992574421
C	9.243241203410	2.633239151026	-0.945363052225
H	9.555451556950	2.125298139193	-1.866537810571
C	10.342133383164	3.615230807049	-0.540458696303
H	11.291977924806	3.102285154987	-0.363574735420
H	10.504244861446	4.366754812874	-1.317841672862
H	10.068971469909	4.142276633696	0.380393681413
C	7.932679024170	3.365754108424	-1.229689405206
H	7.155263965221	2.681352716200	-1.577094953823
H	7.565574426630	3.863848340886	-0.324810471398
H	8.074576219027	4.131765880941	-1.996785913046

FBT-Se₂Th₂



E=−7465.60279162 ($N_{\text{img}} = 0$)

C	4.839336608349	0.257592886700	−0.759844975067
C	3.431188703701	0.327968815249	−0.569536913172
C	2.718422367778	−0.443854405869	0.303058492154
C	3.549651536524	−1.368991599699	1.037195839430
C	4.984687850203	−1.440988353284	0.842795893678
C	5.678396058897	−0.592779800489	−0.098154951553
N	5.557343796962	−2.355039879521	1.614354190354
N	3.114558717724	−2.231921149540	1.945175044290
S	4.394985543848	−3.054226569110	2.498269173766
F	2.817793709554	1.238232517085	−1.332735236278
F	5.313944034289	1.114747814697	−1.669217149269
C	1.272048612155	−0.349006244986	0.474781749348
C	0.488657433798	−1.089224455702	1.320709388520
C	−0.894576053269	−0.783055302708	1.309377006606
H	0.908099983486	−1.848555660908	1.962638379110
C	−1.275262779912	0.216393882496	0.460914980986
H	−1.605976005405	−1.291212118385	1.949084567792
C	7.122263390024	−0.641327990276	−0.316037362434
C	8.025685983236	−1.461519084705	0.307775637274
C	9.380267002772	−1.305051935841	−0.091868308501
H	7.718967986194	−2.178103427703	1.054050029417
C	9.589802005798	−0.358545059189	−1.042000159743
H	10.180795781624	−1.898025194692	0.331980683086
H	10.532300267494	−0.075941977356	−1.487481944581
C	−2.630401658970	0.706943707848	0.238476206221
C	−3.110955765886	1.994235478179	0.212890442650
S	−3.905119377791	−0.448127345357	−0.008600691653
C	−4.518958134044	2.028824112911	0.019692554949
C	−5.100692828954	0.797910058121	−0.105105155865
H	−5.088362024965	2.950280385797	0.009713937956
C	−6.503682384609	0.471138315715	−0.304875382948
C	−7.189512754276	−0.633310119152	0.117754525952
S	−7.551504228087	1.539629111758	−1.180963996188
C	−8.567344009054	−0.632585529609	−0.248099595304

C	-8.896878429702	0.492373243779	-0.945055282752
H	-9.865801258001	0.764946715361	-1.337348695862
C	-2.292275707672	3.231202898668	0.472531705336
H	-1.449454895176	3.285817185043	-0.222983850118
H	-2.912124899414	4.111021730480	0.265562611311
C	-1.759147489241	3.327688868151	1.913755742862
H	-1.150693598550	2.435722174526	2.102773392209
C	-2.900909408475	3.348570267095	2.928587145291
H	-3.523845053400	2.454128479652	2.848090513882
H	-2.513292235341	3.400041432204	3.949585229228
H	-3.543502961822	4.222323270380	2.770001550153
C	-0.861234640058	4.554500604140	2.059535073295
H	-1.423229903545	5.473943385026	1.860622625536
H	-0.454579097595	4.625357593555	3.071959745057
H	-0.020718542147	4.514944593484	1.360606522843
H	-6.730139930191	-1.423422918755	0.699283546816
C	-9.525702915493	-1.748999637704	0.060806727587
H	-10.514318992639	-1.329837564462	0.273488217367
H	-9.202151991767	-2.263092744719	0.973913323438
C	-9.659921058833	-2.785566432545	-1.071054920952
H	-9.992563999206	-2.246928855161	-1.967305750691
C	-10.722746423368	-3.822816128000	-0.709975055173
H	-11.689322996456	-3.351953384827	-0.508391696074
H	-10.861035284177	-4.543252912355	-1.520687644877
H	-10.428584556479	-4.381535291022	0.185387853592
C	-8.325627112727	-3.458112421787	-1.390955796953
H	-7.573494047252	-2.731634889384	-1.707171641292
H	-7.938768719745	-3.984542299763	-0.510677766350
H	-8.443167014762	-4.192217641288	-2.192591203008
Se	8.017259481885	0.472103275281	-1.552883845156
Se	0.198522001123	0.875098498378	-0.482020503944

Reference

1. J.-F. Jheng, Y.-Y. Lai, J.-S. Wu, Y.-H. Chao, C.-L. Wang and C.-S. Hsu, *Adv. Mater.*, 2013, **25**, 2445.
2. Gaussian 09, Revision **A.1**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, Jr., J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.