Supporting Information for

Structure-function relationships of high-electron mobility naphthalene diimide copolymers prepared by direct arylation

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Instrumentation.

NMR spectroscopy. ^{1}H (500.13 MHz) and ^{19}F (470.59 MHz) NMR spectra were recorded on a Bruker Avance III spectrometer using a 5 mm ^{1}H/^{13}C/^{19}F/^{31}P gradient probe. The polymer spectra were recorded at 393 K using $C_2D_2Cl_4$ as solvent. The ^{1}H NMR spectra were referenced to the residual solvent peak (δ(^{1}H) 5.98 ppm). The ^{19}F NMR spectra were referenced to external C_6F_6 (δ(^{19}F) -163.0 ppm). ^{1}H NMR monomer spectra were recorded at 300 MHz and ^{13}C NMR spectra at 75 MHz at room temperature in $CDCl_3$ (δ(^{1}H) 7.26 ppm; δ(^{13}C) 77.0 ppm).

GPC measurements were carried out on four SDV gel 5 μm columns, with pore sizes ranging from 10^3 to 10^6 Å (PSS), connected in series with a Knauer K-2301 RI detector, and calibrated with polystyrene standards. $CHCl_3$ was used as eluent at room temperature at a flow rate of 1.0 mL/min.

UV-Vis measurements were carried out on a Perkin Elmer λ1050 spectrophotometer, using a tungsten lamp as the excitation source.

CV measurements were carried out using an Autolab PGSTAT101 potentiostat of Eco-Chemie (Utrecht, The Netherlands), run by a PC with the NOVA 1.6 in a 4 cm^3 cell equipped with a presaturator. The working electrode was a 0.071 cm^2 glassy carbon disk embedded in Teflon® of Amel (Milan, Italy), the counter electrode was a Platinum wire and the operating reference electrode was an aqueous saturated calomel one (SCE). All the measurements were performed in 0.1 M $TBAPF_6$ solution of acetonitrile.

Photo Electron Spectroscopy in Air (PESA) measurements were made using a Riken Keiki AC-2 spectrometer. A power intensity of 5nW was used and all data were plotted using a power number of 0.5.

Differential scanning calorimetry (DSC) was carried out on a DSC Pyris 1 from Perkin Elmer at 10 K/min under nitrogen. Glass transition temperatures were taken from the second heating curves after baseline substraction, the mass of the samples was ~10-15 mg.

Thermogravimetric analysis (TGA) was carried out on a STA instrument 409 from Netzsch between 50−650 °C at 10 K/min under nitrogen.

Density Functional Theory (DFT) calculations.

P(ThNDIThF$_4$), **4**, and P(FuNDIFuF$_4$), **5**, were modeled following two procedures.

First only the *monomeric unit* of **4** and **5** was considered in order to explore all possible stable conformers, in particular with regard to the dihedral angles between the NDI and Fu/Th units and Fu/Th and F_4 moieties (see Figure S4). The molecular and electronic structures were optimized at the Density Functional Theory (DFT) level, considering three exchange

correlation functionals, namely B3LYP, ωB97XD (as implemented in G09) and LC-BLYP with the polarized split-valence basis set 6-31G**. B3LYP was considered because one of the standard DFT functional used in literature, ωB97XD and LC-BLYP to explore the effects introduced by dispersion forces and range-separation parameter.[1]

In the case of LC-BLYP, the range-separation parameter was optimized at $\mu = 0.2\ a_0^{-1}$ by minimizing the $J(\mu)$ function ($J(\mu) = |\varepsilon_H^{\mu}(N) + E_{gs}^{\mu}(N-1) - E_{gs}^{\mu}(N)|$, with ε_H denoting the HOMO energy of the N electron system, $E_{gs}^{\mu}(N-1)$ the total ground state energy of the $N-1$ electron system, and $E_{gs}^{\mu}(N)$ the total ground state energy of the N electron system.[2,3]

For the monomer of **4** we obtained J(0.2) = 0.03 eV, for **5** J(0.2) = 0.06 eV, values comparable to those reported in literature for similar donor-acceptor polymer and DFT benchmarking studies.[4]

In each case, equilibrium geometries were validated through harmonic frequency calculations; no imaginary values were found.

Figure S4 reports the DFT relaxed potential energy profiles for both systems along the two principal dihedral coordinates (τ_1 and τ_2, see Figure S4). All DFT functionals predict qualitatively similar results, with some differences in the value of the rotational barriers. P(FuNDIFuF$_4$) has two stable non-equivalent minima (*syn* and *anti*) for τ_1 in the range between 20°-30° (LC-BLYP < B3LYP < ωB97XD) and 140° respectively, while there are two stable equivalent minima for τ_2 in the range of 0°-20° (or 180°-160°). Rotational barriers for converting one minimum to the other one (both for τ_1 and τ_2) are around 3-5 kcal/mol (B3LYP < ωB97XD < LC-BLYP). Similar results were obtained for the case of P(Th-NDI-Th-F$_4$), however τ_1 shows higher equilibrium values ranging from 30°-60° (or 140°-120°, LC-BLYP < B3LYP < ωB97XD) than the furan-based copolymer. P(ThNDIThF$_4$) features higher

τ_1 values (30°-60° *vs* 20°-30°) and higher rotational barriers (2-6 kcal/mol vs. 0.2-0.6 kcal/mol) than P(FuNDIFuF$_4$).

Generally, ωB97XD predicts more distorted structures and higher rotational barriers than B3LYP and LC-BLYP.

Recent systematic structural investigations and vibrational analysis carried out on a similar donor-acceptor copolymer, as P(NDI2OD-T2)[5], demonstrate that minima and rotational potential barriers obtained at the MP2 level match the ones computed at the B3LYP level of theory.[6] Moreover the ground state structure and the torsional angle between NDI and T2 unit computed for P(NDI2OD-T2) at the B3LYP/6-31G** level match the one *experimentally* derived from vibrational spectra.[5] In this regard, *ground state geometries and force field* computed at the B3LYP level, even for this class of donor-acceptor materials, can be considered reliable. Range separated hybrid functionals can overestimate ground state torsional angles and rotational barriers, although they are *essential* in the evaluation of the ground and excited state electronic structure.

For this reason along the main manuscript we report B3LYP optimized structures for the monomers of **4** and **5** species.

The LC-BLYP (with μ parameter at 0.2 a_0^{-1}) optimized ground state structures (minima) and rotational barriers do not much differ from the B3LYP ones.

The second approach consisted in studying *long oligomers* (four repeat units) of **4** and **5**, the structures of those were fully optimized at the B3LYP and LC-BLYP (μ = 0.2 a_0^{-1})/6-31G** level. The structures of **4** and **5** tetramers, as reported in Figure S5 do not differ significantly and both functionals predict a planar geometry for **4** and a straight geometry for **5**.

As expected, range separated functional is relevant for the prediction of the electronic and optical properties. In Figure S6, the computed TDDFT vertical transition energies for the

tetramers of **4** and **5**. LC-BLYP ($\mu = 0.2\ a_0^{-1}$) well match the experimental UV-Vis absorption spectra, thus validating also the ground state structure obtained for the tetramer of **4** and **5**.

Intra-molecular reorganization energies (λ) were computed *via* the Adiabatic Potential approach.[7] For instance, the hole reorganization energy is defined as:

$$\lambda = \lambda^{(1)}_{rel} + \lambda^{(2)}_{rel}$$

with

$$\lambda^{(1)}_{rel} = E^{(1)}(M+\cdot) - E^{(0)}(M+\cdot)$$

$$\lambda^{(2)}_{rel} = E^{(1)}(M) - E^{(0)}(M)$$

$E^{(0)}(M+\cdot)$ and $E^{(0)}(M)$ are the ground-state energies of the cation and the neutral molecule, $E^{(1)}(M+\cdot)$ is the energy of the cation at the optimal geometry of the neutral molecule, and $E^{(1)}(M)$ is the energy of the neutral molecule at the optimal geometry of the cation. The electron reorganization energy is defined analogously.

The unrestricted DFT approach was used for the geometry optimizations of both cationic (hole) and anionic (electron) species for each functional (namely B3LYP, ωB97XD, and LC-BLYP). For monomers, all three DFT functional were considered in the calculation of reorganization energies; for tetramer, only LC-BLYP ($\mu = 0.2\ a_0^{-1}$) was considered. A detailed DFT benchmark regarding reorganization energies is currently ongoing, and it is out of the scope of the present investigation.

Table S2 compares intra-molecular electron and hole reorganization energies for each XC functional tested. Electron reorganization energies are lower than hole reorganization energies (at each level of theory), confirming the *n*-type character of **4** and **5**.

The range-separated functionals (ωB97XD and LC-BLYP) predict, at the monomer level, higher reorganization energies than the hybrid functional (B3LYP)[8], however the trends are the same.

Electron reorganization energies for tetramer of **4** and **5** were computed at the LC-BLYP (μ = 0.2 a_0^{-1}) level, because the well performance of this functional in predicting the electronic structure of ground and excited states (Figure S6). Values are reported in the same Table.

As a quantitative comparison, we report the computed (B3LYP) reorganization energies for the monomer of P(NDI2OD-T2) a well performing *n*-type semiconductors. Electron reorganization for the monomers of **4** and **5**, at the B3LYP level, are similar to that of P(NDI2OD-T2), thus confirming the good *n*-type character of the synthesized copolymers. All calculations were performed using Gaussian 09 program.[9]

FET fabrication and measurements: We adopted a top-gate, bottom-contact architecture for optimized device performance. Thoroughly cleaned 1737F glass was used as the substrate. Interdigitated Au contacts were defined by a lift-off photolithographic process with a 0.7 nm thick Cr adhesion layer. The thickness of the Au contacts was 30 nm. Substrates were cleaned in a sonic bath in isopropyl alcohol for 2–3 min before deposition of the semiconductor. After filtering through a 0.2 μm polytetrafluoroethylene (PTFE) filter, solutions of the polymeric semiconductors of this work (5 g L^{-1} in toluene) were deposited by spin-coating at 1000 rpm for 30 s in a nitrogen glove box. The semiconductor was then annealed on a hot plate in a nitrogen atmosphere at temperatures ranging from 100 °C to 350 °C. PMMA (Sigma-Aldrich) with M_w = 120 kg mol^{-1} was spun from n-butanone (65 g L^{-1} , filtered with a 0.2 μm PTFE filter) in air at 1300 rpm for 60 s. Dielectric-layer thicknesses ≈660 nm were obtained. After the dielectric deposition, the devices were annealed under nitrogen, on a hot-plate, at 120 °C for 14 h. 30 nm thick gate Al electrodes were thermally evaporated as gate contacts. The electrical characteristics of the transistors were measured in a nitrogen glove-box on a Wentworth Laboratories probe station with an Agilent B1500A semiconductor device analyzer. Saturation effective electron mobilities were extracted from the derivative of the plot of $I_d^{1/2}$ vs. V_g following the gradual channel approximation for FETs.

GIWAXS measurements were performed at the SAXS/WAXS beamline of the Australian Synchrotron.[10] 9 keV Photons were used with 2D scattering patterns recorded on a Pilatus 1M detector. The sample-to-detector distance was calibrated using a silver behenate standard. Scattering patterns were recorded as a function of X-ray angle of incidence, with the angle of incidence varied from 0.05 degrees below the critical angle of the organic film to 0.2 degrees above the critical angle. The images reported were at the critical angle as identified by the angle with the highest scattering intensity. Data acquisition times of 3s were used, with three 1 s exposures taken with offset detector positions to cover gaps in the Pilatus detector. X-ray diffraction data are expressed as function of the scattering vector, q, that has a magnitude of $(4\pi/\lambda)\sin(\theta)$, where θ is half the scattering angle and λ is the wavelength of the incident radiation. NEXAFS measurements were performed at the Soft X-ray Spectroscopy Beamline at the Australian Synchrotron.[11] Nearly perfectly linearly polarized photons ($P \approx 1$) from an undulator X-ray source with high spectral resolution ($E/\Delta E \leq 10\ 000$) were focused into an ultrahigh vacuum chamber to a ~0.4 × 1 mm spot size. X-ray absorption was measured using the partial electron yield method where x-ray absorption is measured by detecting photoelectrons emitted from the surface with a channelplate detector with a pass energy of 202.5 eV. A fresh spot on the sample was used for each spectrum with the acquisition time minimised (0.5 s per 0.1 eV step) to prevent beam damage. The recorded signals were normalized to the incident photon flux using the "stable monitor method," in which the sample signal is compared consecutively to a clean reference sample and the time variation in flux is measured via a gold mesh.[12] The normalized spectra were scaled by normalising the pre-edge (at 280 eV) to zero and the post-edge (at 320 eV) to one, effectively normalizing to the total carbon content of the material. The photon energy was calibrated by measuring the NEXAFS spectrum of highly oriented pyrolytic graphite simultaneously to the sample signal and normalising to the exciton peak at 291.65 eV.[13] Average tilt angles of the conjugated

backbone were determined by peak fitting and determining the average tilt angle of the associated transition dipole moment using the equation:

$$I = \frac{1}{3}\left[1 + \frac{1}{2}\left(3\cos^2\theta - 1\right)\left(3\cos^2\gamma - 1\right)\right] \quad (1)$$

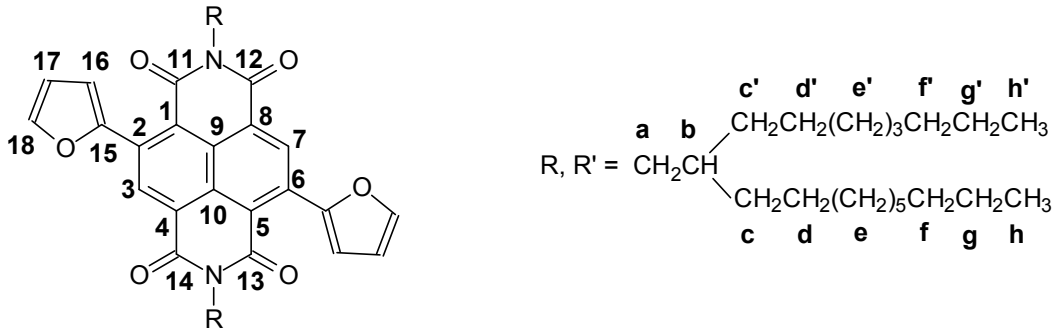
where I is the resonance intensity (proportional to the area under the peak), θ the angle of incidence and γ the average tilt angle of the transition dipole moment (measured with respect to the surface normal). The tilt angle of the conjugated backbone with respect to the surface normal is then $\alpha = 90^\circ - \gamma$.

General description of chemicals

All chemicals and solvents were purchased from Aldrich and used as received unless otherwise noted. $NDIBr_2$ and ThNDITh were prepared according to the literature.[14] PivOK was prepared from an equimolar mixture of pivalic acid and potassium hydroxide in water and stirred at room temperature overnight. The precipitate was filtered off, washed with water and dried under vacuum at 60 °C.

Synthesis

Synthesis of FuNDIFu. 2,6-Dibromonaphthalene-1,4,5,8-tetracarboxylic-N,N‘-bis(2-octyldodecyl)diimide (298.2 mg, 0.3 mmol) and 2-tributylstannylfuran (221. 8 mg, 0.6 mmol, 2.1 eq) were degassed in THF (10.0 ml) with nitrogen for 20 minutes. Afterwards $Pd_2(dba)_3$ (5.7 mg, 6.3 x 10^{-3} mmol, 2.1 mol%) and triphenylphosphine (8.7 mg, 3.3 x 10^{-2} mmol, 11.2 mol%) were added and the mixture was degassed again for 20 minutes. The mixture was heated at 80 °C for 17 hours under an inert gas atmosphere. After cooling to room temperature, the solvent was removed under reduced pressure and the crude product was filtered eluted with DCM over a short plug of SiO_2. After removing the DCM, the product (271.2 mg, 0.3 mmol, 96 %) was purified by recrystallization from ethanol.



^{1}H NMR (300 MHz, $CDCl_3$): 9.04 (s, 2H, $H_{3/7}$), 7.67 (d, ^{3}J = 1.5 Hz, 2H, H_{18}), 7.31 (d, ^{3}J = 3.4 Hz, 2H, H_{16}), 6.63 (dd, ^{3}J = 1.5 Hz, ^{3}J = 3.4 Hz, 2H, H_{17}), 4.13 (d, J = 7.3 Hz, 4H, H_a), 1.99 (m, 2H, H_b), 1.5-1.1 (64H, $H_{c\text{-}g,c'\text{-}g'}$), 0.86 ppm (12H, $H_{h,h'}$).

^{13}C (75 MHz, $CDCl_3$): 162.7 ($C_{12/14}$), 162.6 ($C_{11/13}$), 150.8 (C_{15}), 144.6 (C_{18}), 134.5 ($C_{2/6}$), 134.1 ($C_{3/7}$), 127.2 ($C_{9/10}$), 125.8 ($C_{4/8}$), 121.1 ($C_{1/5}$), 114.6 (C_{16}), 112.4 (C_{17}), 45.1 (C_a), 36.6 (C_b), 31.8 and 31.7 ($C_{f,f'}$), 31.7 ($C_{c,c'}$), 30.0 – 29.3 ($C_{e,e'}$), 26.4 ($C_{d,d'}$), 22.6 ($C_{g,g'}$), 14.1 ppm ($C_{h,h'}$).

General protocol of µW-direct arylation polycondensation. Potassium pivalate (42.07 mg, 3.0 x 10^{-4} mol, 3.0 eq) and the monomers 2,6-bis(2-furyl)naphthalene-1,4,5,8-tetracarboxyl-N,N'-bis(2-octyldodecyl)diimide (95.94 mg, 1.0 x 10^{-4} mol, or the corresponding amount of ThNDITh and 1,4-dibromotetrafluorobenzene (30.79 mg, 1.0 x 10^{-4} mol), as 0.1 M solutions from a 1:1 mixture of chlorobenzene and N,N'-dimethylacetamide, were placed in a microwave glass vial. The mixture was degassed with argon for 20 minutes, $Pd(OAc)_2$ (1.80 mg, 8.0 x 10^{-6} mol, 8.0 mol-%) was added and the mixture was degassed again for 20 min. The mixture was heated in the microwave reactor for 2 hours at 100 °C (50 W). After the reaction was completed, the mixture was cooled to room temperature, diluted with THF, precipitated into methanol and filtered. The polymers were Soxhlet extracted with methanol, acetone, ethyl acetate, *iso*-hexane, and chloroform. The chloroform fractions were filtered, concentrated, collected, and finally dried at 40 °C overnight.

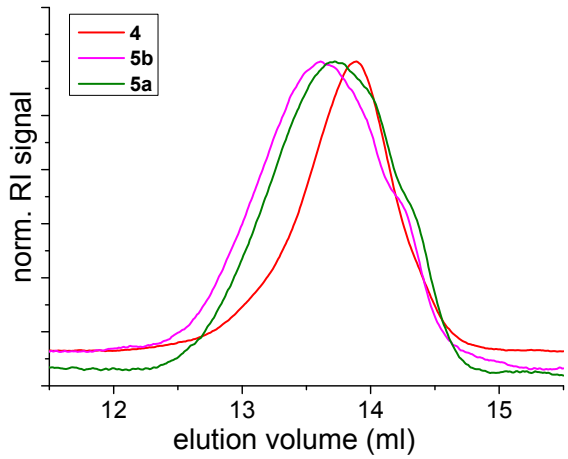


Figure S1. SEC in trichlorobenzene at 150 °C.

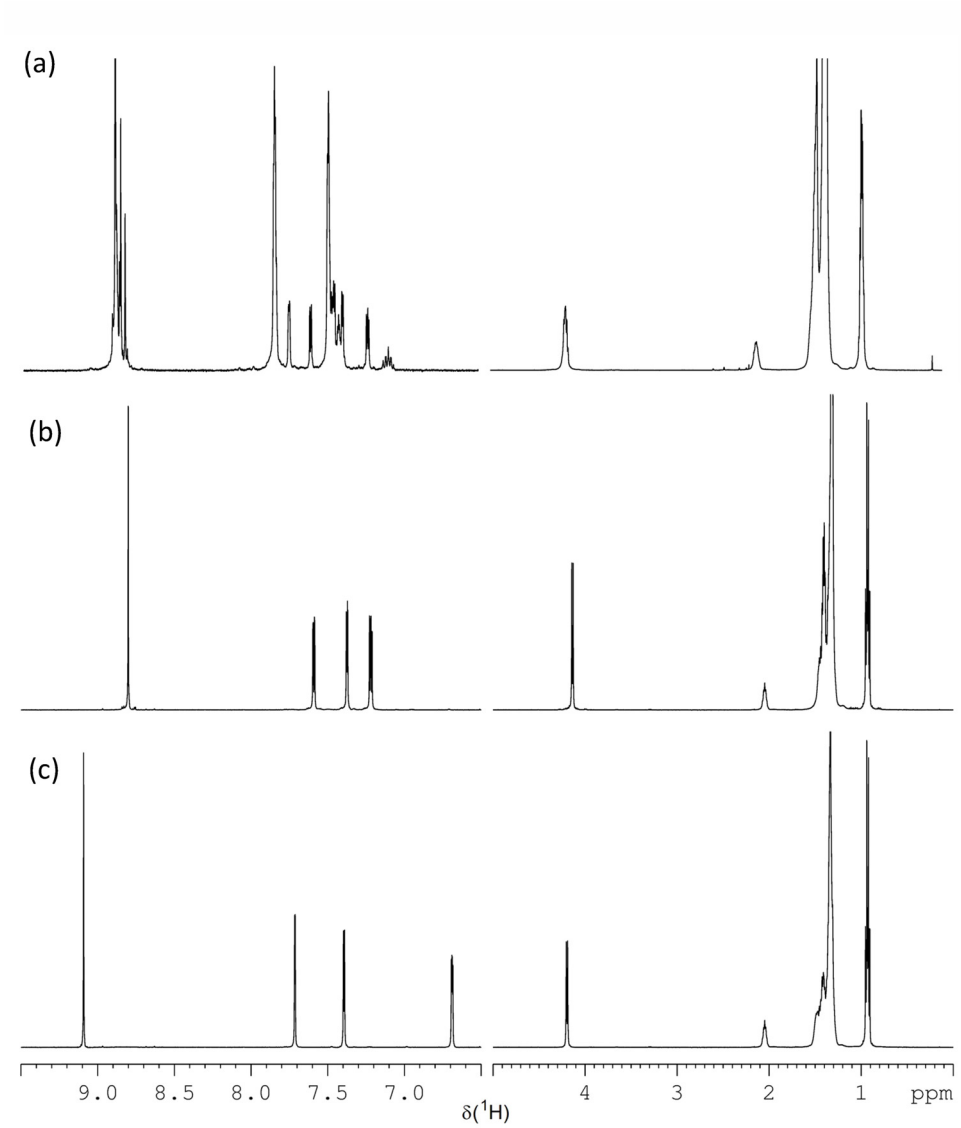


Figure S2. ^{1}H NMR spectra ($C_2D_2Cl_4$, 120 °C) of P(ThNDIThF$_4$) **5a** (a), ThNDITh monomer **2a** (b), and FuNDIFu monomer **1** (c).

Table S1. Energies of the shoulder (sh) and the maximum in UV-Vis spectra of P(FuNDIFuF$_4$) and P(ThNDIThF$_4$) in solution (S) and solid state film (F).

		Low energy CT band (nm)		High energy band (nm)		
P(FuNDIFuF$_4$)	S	591 (sh)	545	389 (sh)	370	351 (sh)
	F	617	573	420 (sh)	394	354 (sh)
P(ThNDIThF$_4$)	S	-	518	385 (sh)	366	348
	F	646 (sh)	585	394 (sh)	365	

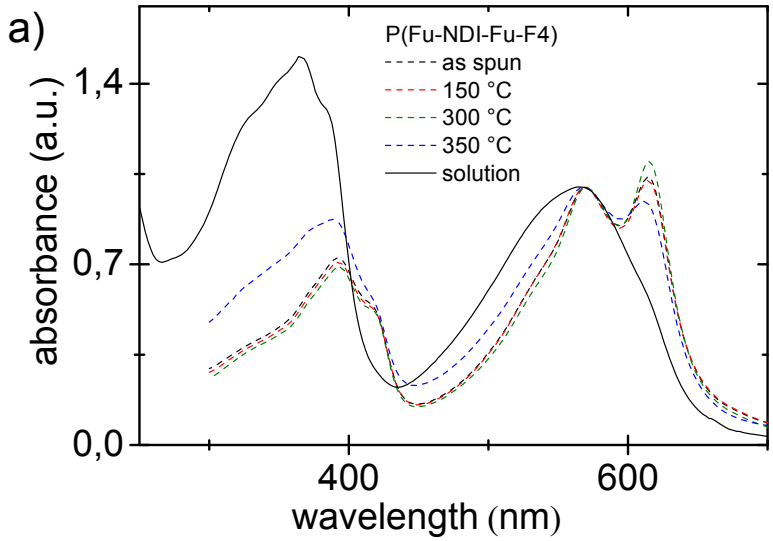


Figure S3. Temperature-dependent UV-vis of films of **4**

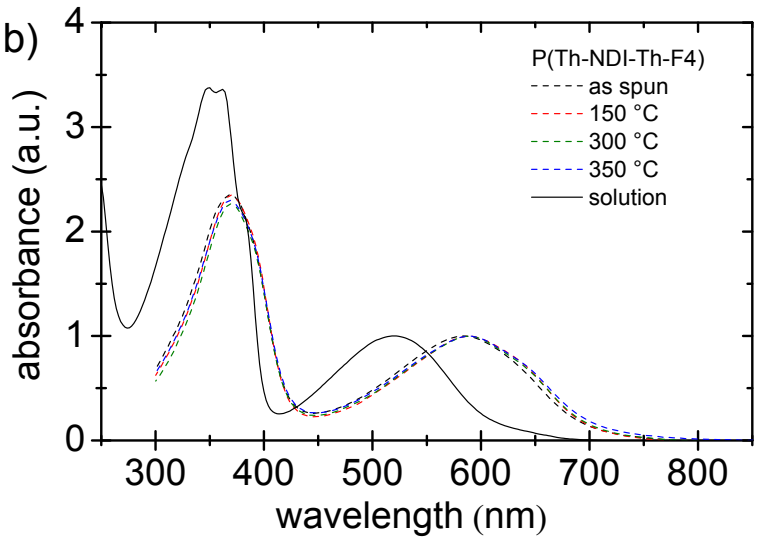


Figure S4. Temperature-dependent UV-vis of films of **5b**.

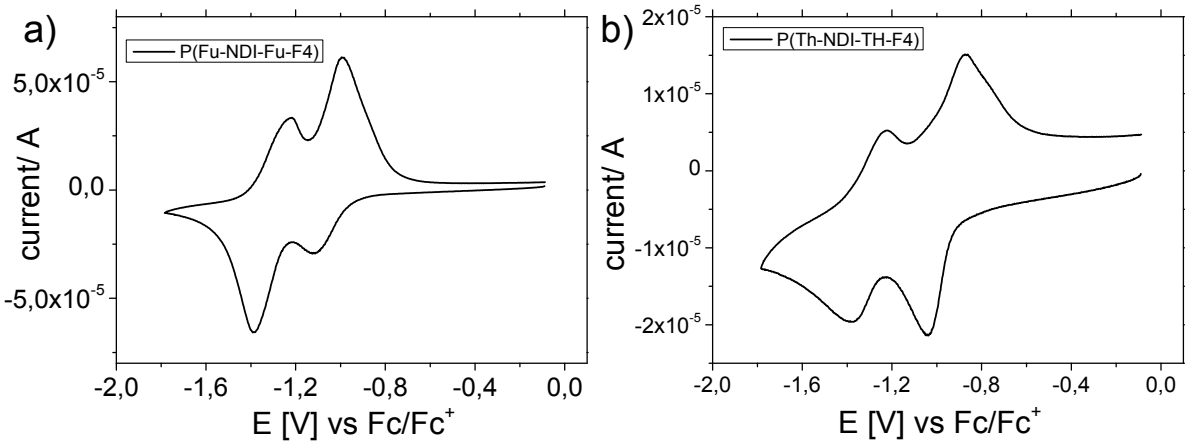


Figure S5. Cyclic voltammetry data of films of a) **4** and b) **5b**. Curves were taken in acetonitrile at 100 mV/s.

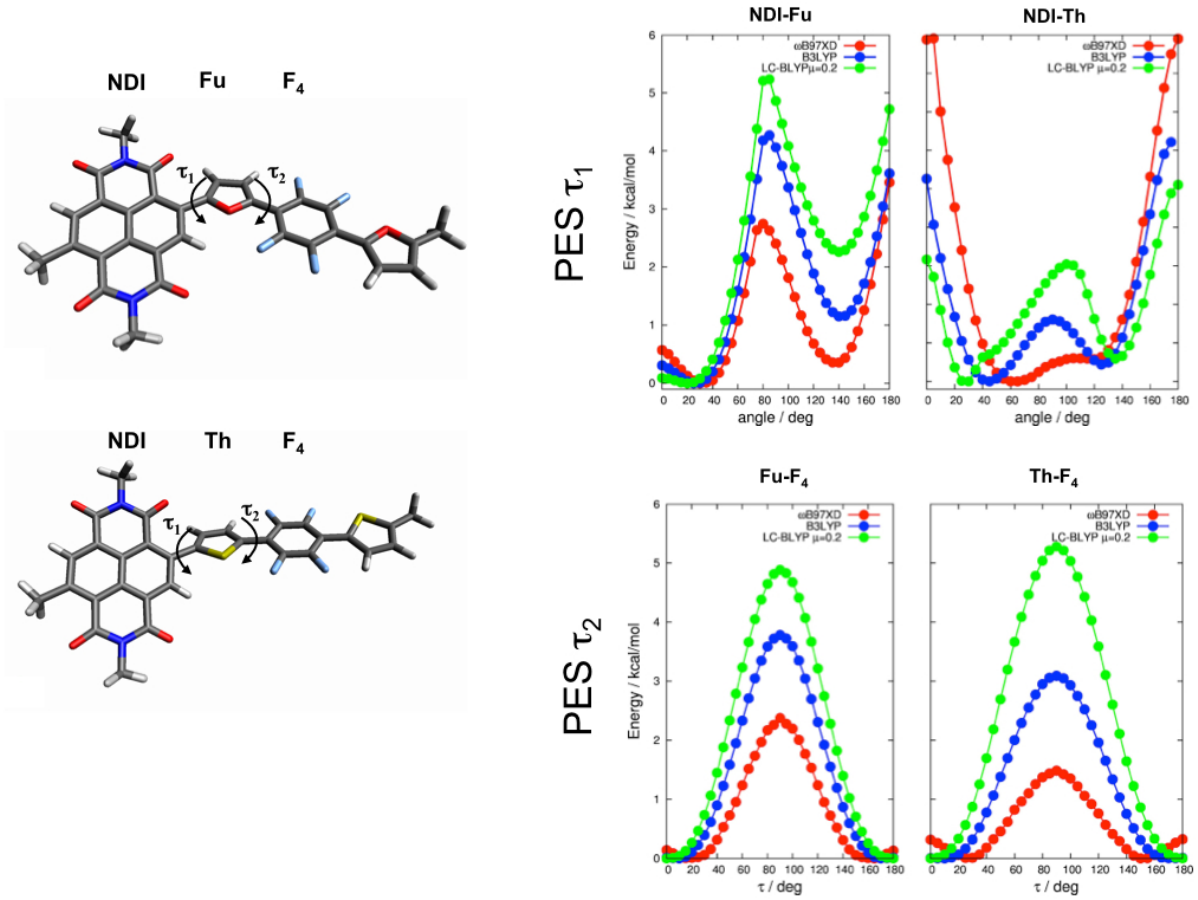


Figure S6. B3LYP, ωB97XD, LC-BLYP ($\mu = 0.2a_0^{-1}$) fully relaxed potential energy profiles for τ_1 and τ_2.

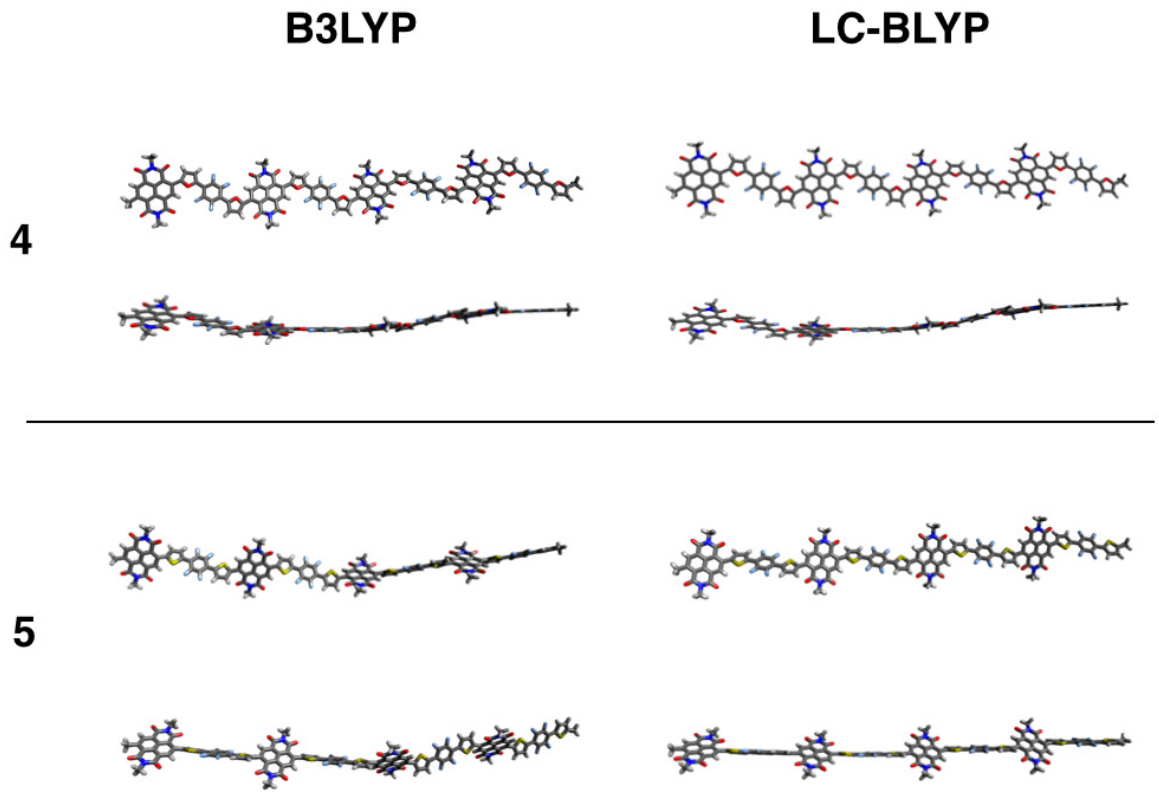


Figure S7 B3LYP and LC-BLYP ($\mu = 0.2a_0^{-1}$) optimized structures for tetramer of **4** and **5**.

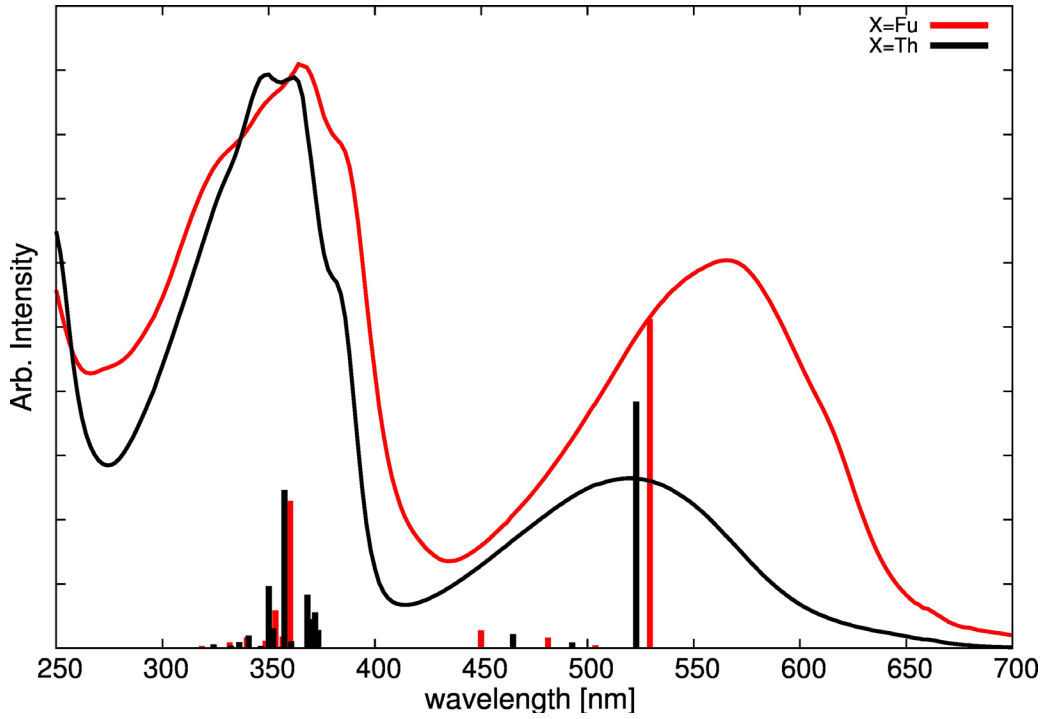


Figure S8 TD-LC-BLYP ($\mu = 0.2a_0^{-1}$) vertical transitions for tetramer of **4** (red sticks) and **5** (black sticks). Solution absorption spectra (see manuscript) for **4** (red line) and **5** (black line).

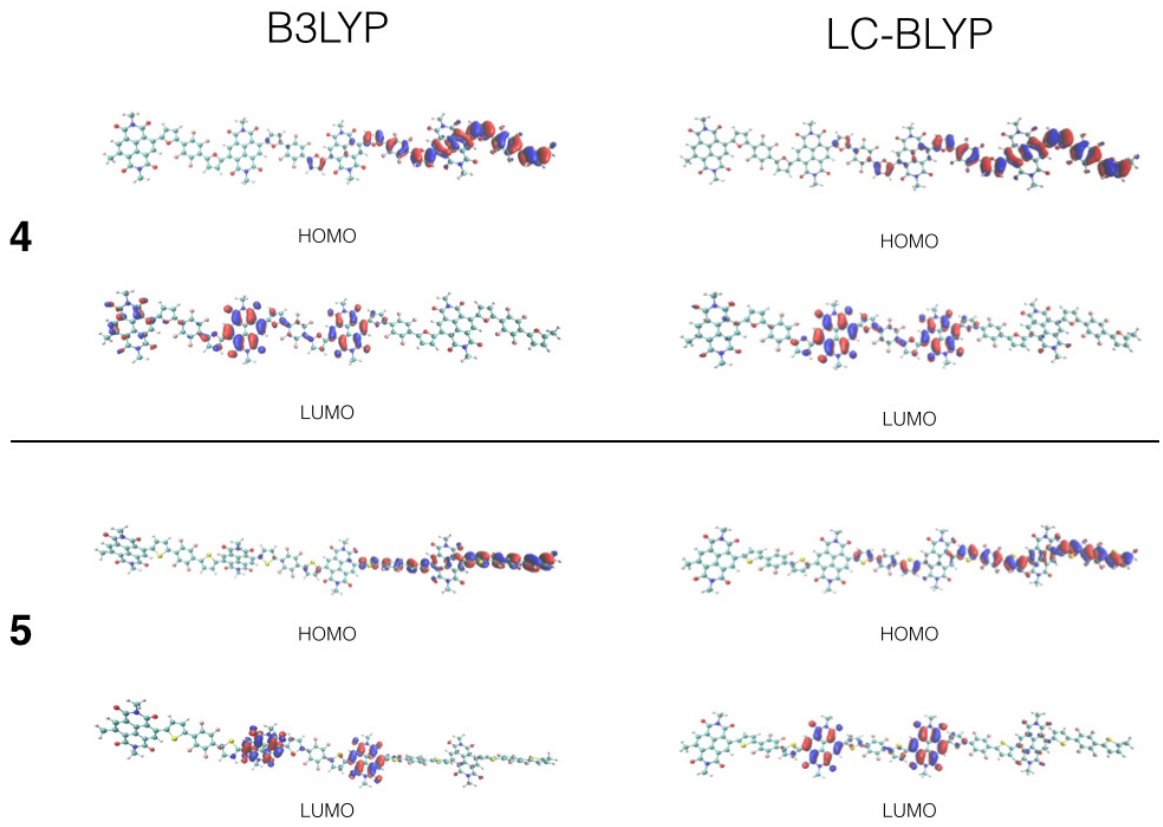


Figure S9 Highest (Lowest) Occupied Molecular Orbitals (HOMO and LUMO) computed at the B3LYP and LC-BLYP ($\mu = 0.2a_0^{-1}$) level for tetramer of **4** and **5**.

Table S2. Hole and electron reorganization energies for all DFT methods employed.

	λ_{elec} (eV)	λ_{hole}(eV)
FuNDIFuF$_4$		
B3LYP	0.27	0.27
LC-BLYP (μ=0.2 a_0^{-1}) *LC-BLYP (μ=0.2 a_0^{-1}) tetramer*	0.32 *0.17*	0.36
ωB97XD	0.40	0.52
ThNDIThF$_4$		
B3LYP	0.27	0.31
LC-BLYP (μ =0.2 a_0^{-1}) *LC-BLYP (μ=0.2 a_0^{-1}) tetramer*	0.32 *0.17*	0.42
ωB97XD	0.41	0.56
P(NDI2OD-T2) *B3LYP*	*0.27*	*0.40*

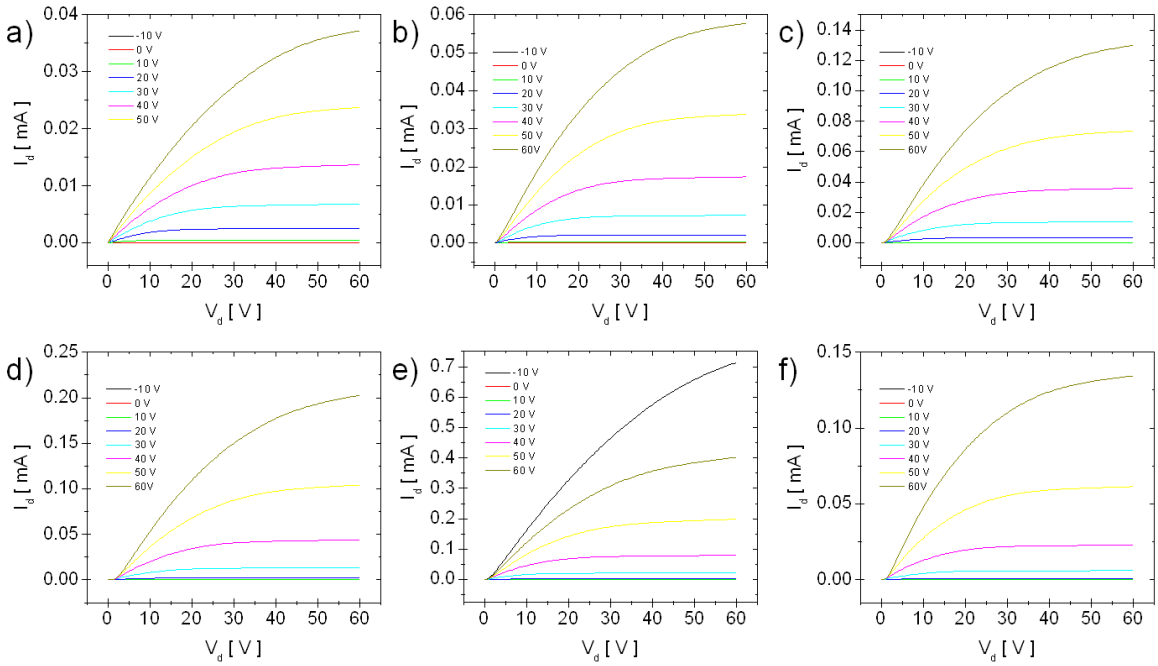


Figure S10. Output curves (I_d vs V_d) of **4** based FETs with 100 °C (a), 150 °C (b), 200 °C (c), 250 °C (d), 300 °C (e) and 350 °C (f) thermal treatment on the semiconductor films.

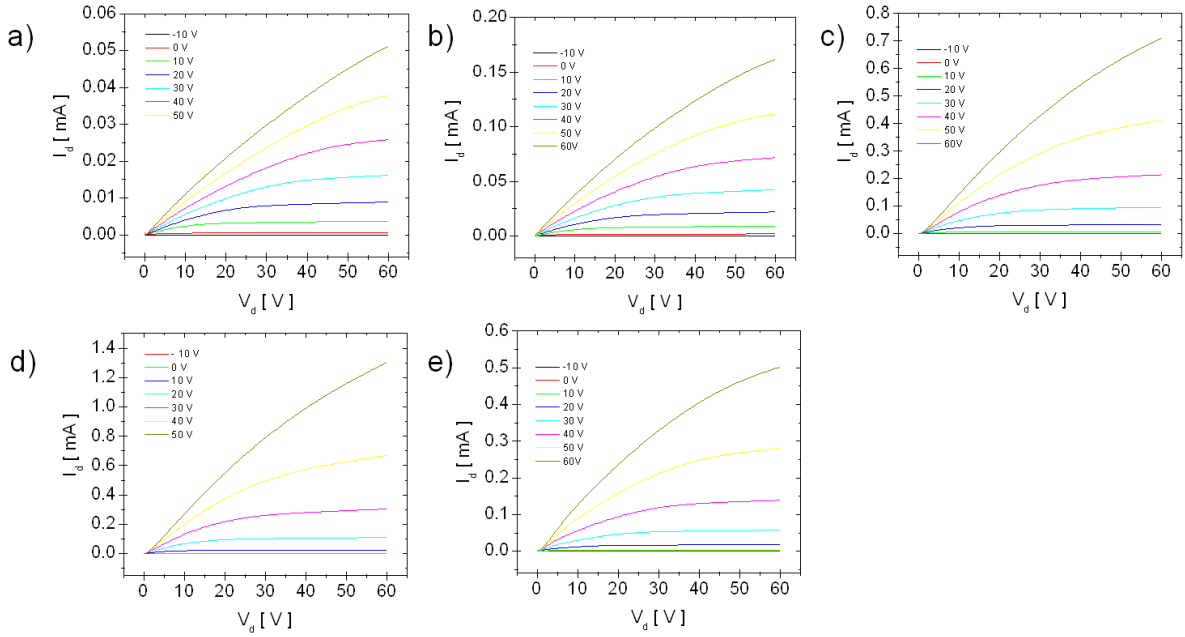


Figure S11. Output curves (I_d vs V_d) of **5b** based FETs with 100 °C (a), 150 °C (b), 200 °C (c), 250 °C (d), 300 °C (e) thermal treatment on the semiconductor films.

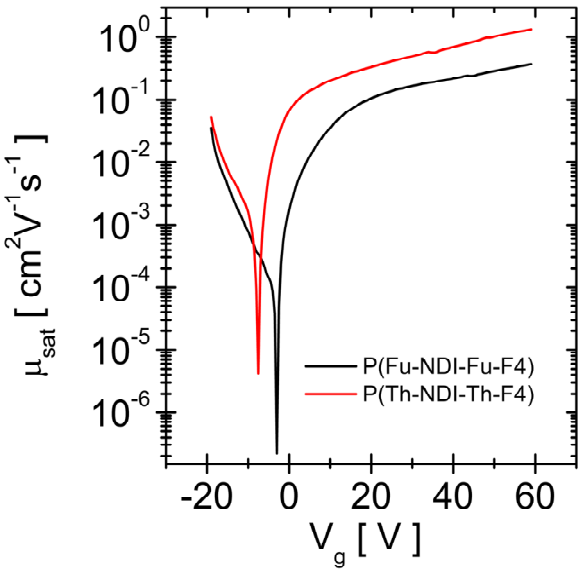


Figure S12. Representative saturation mobilities (μ_{sat}) of **4** and **5b**.

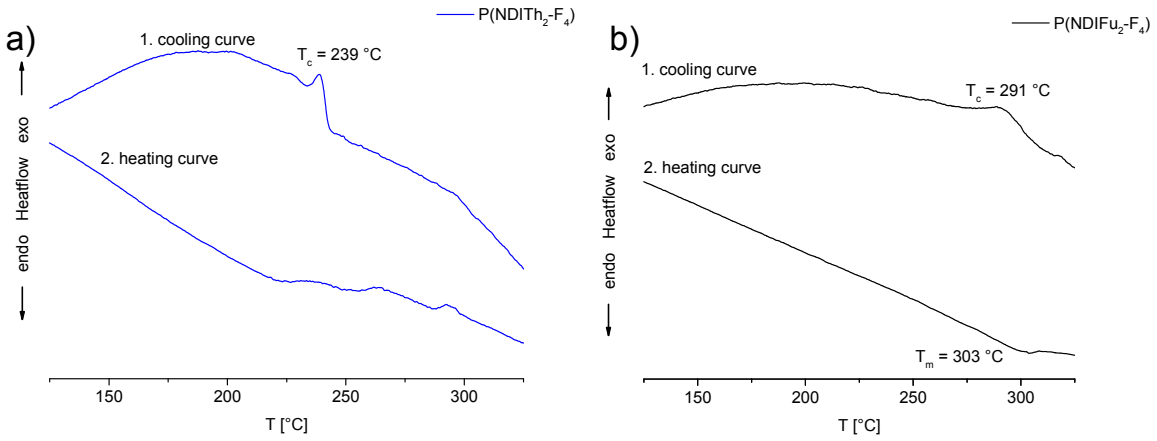


Figure S13. Differential scanning calorimetry of a) **5b** and b) **4**. Curves were taken at 10 K/min under nitrogen, first cooling and second heating curves are shown. From the heating curve of 5b is was not possible to extract a melting temperature.

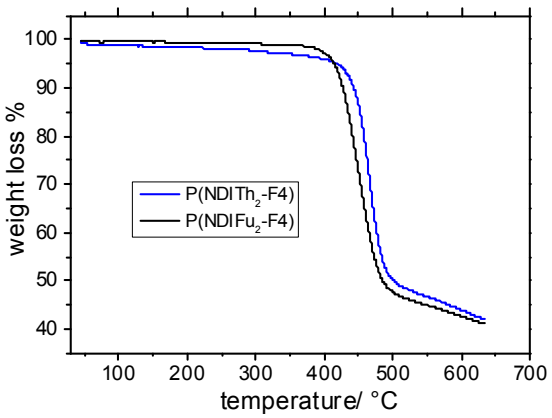


Figure S14. Thermogravimetry of **4** and **5b** at 10 K/min under N_2.

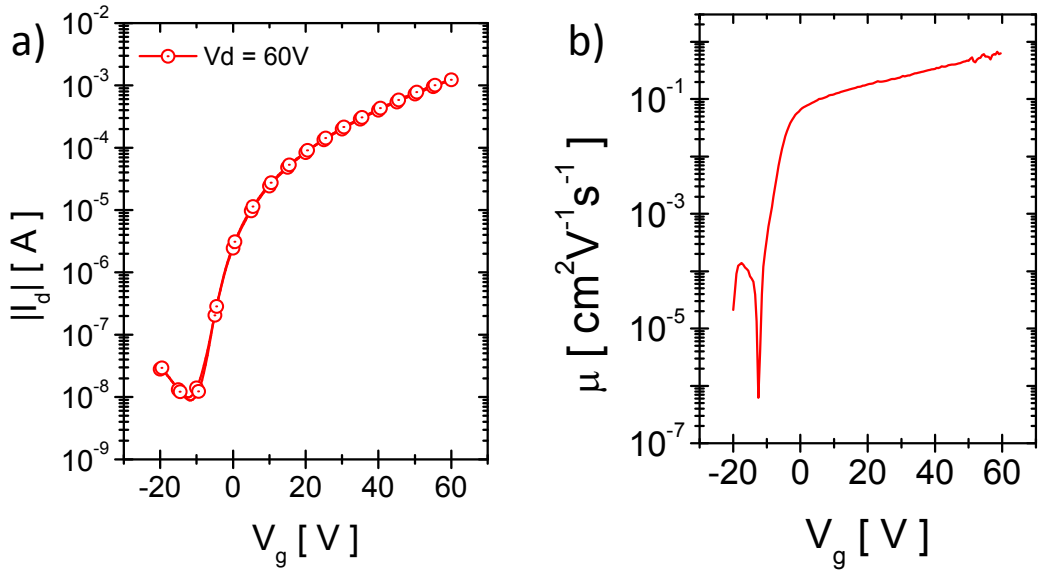


Figure S15. Representative OFET data for P(ThNDIThF$_4$) **5a**. a) Transfer characteristics and b) saturation mobilities.

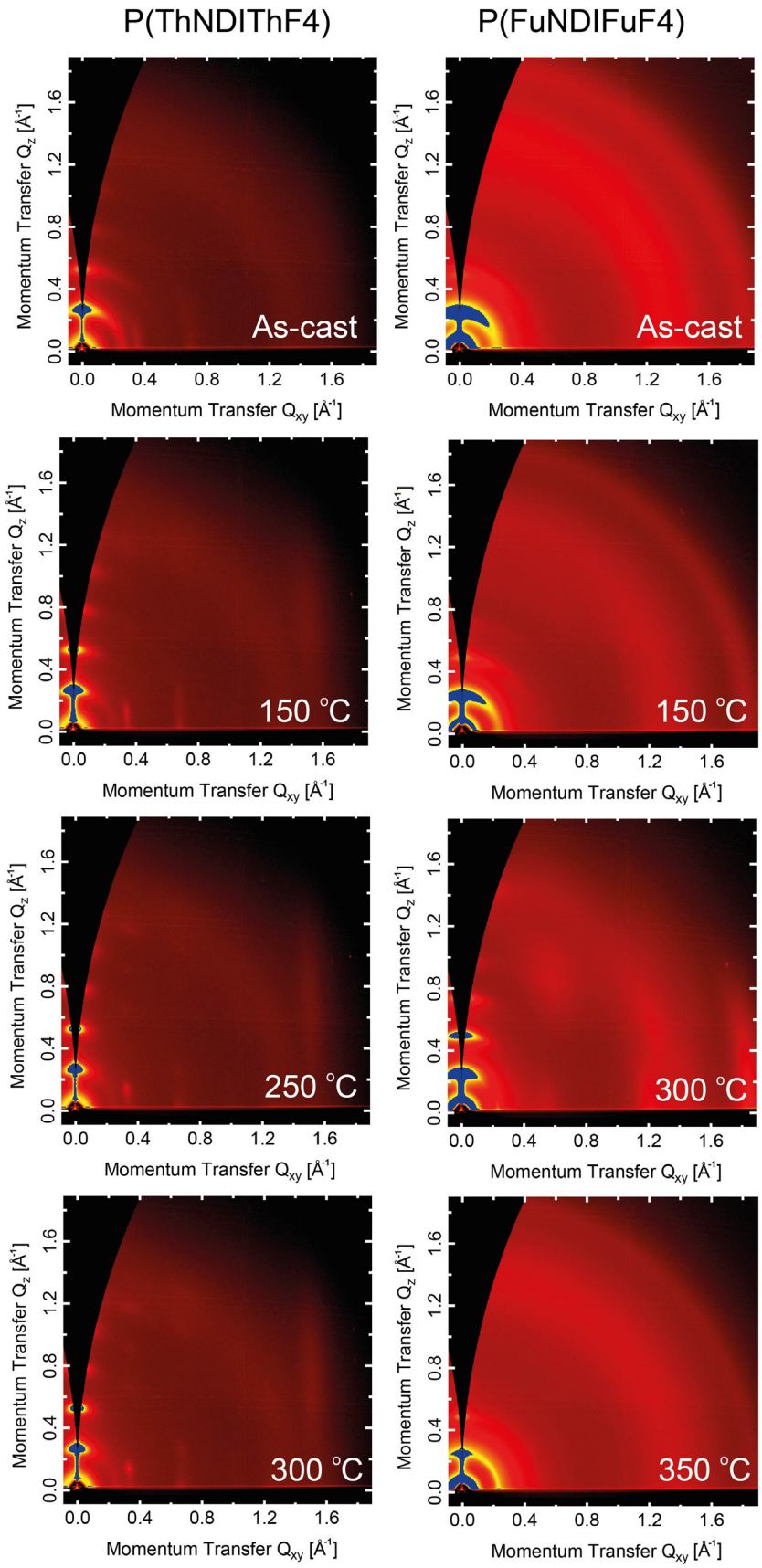


Figure S16. Full 2D GIWAXS data set taken of films prepared with different annealing temperature.

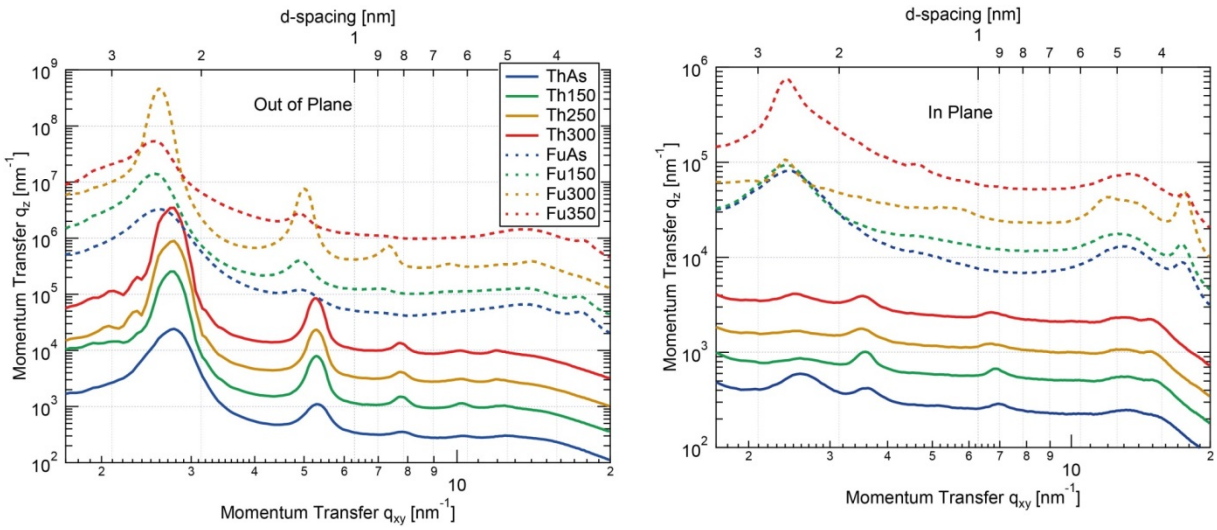


Figure S17. Out-of-plane (left) and in-plane (right) line-outs taken from the 2D GIWAXS data for **4** (Fu) or **5b** (Th).

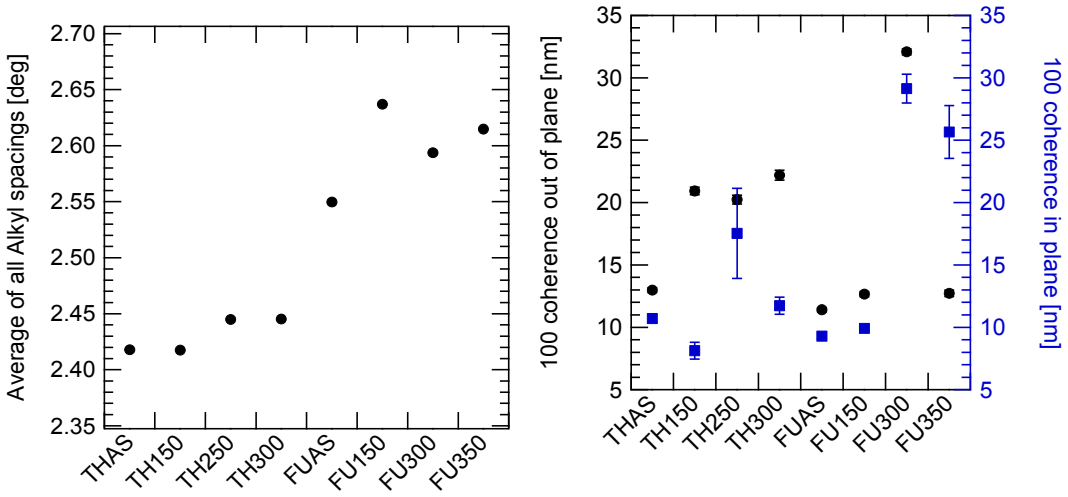


Figure S18. (100) alkyl spacing, left, and (100) coherence length, right, as a function of **4** (Fu) or **5b** (Th) and annealing temperature.

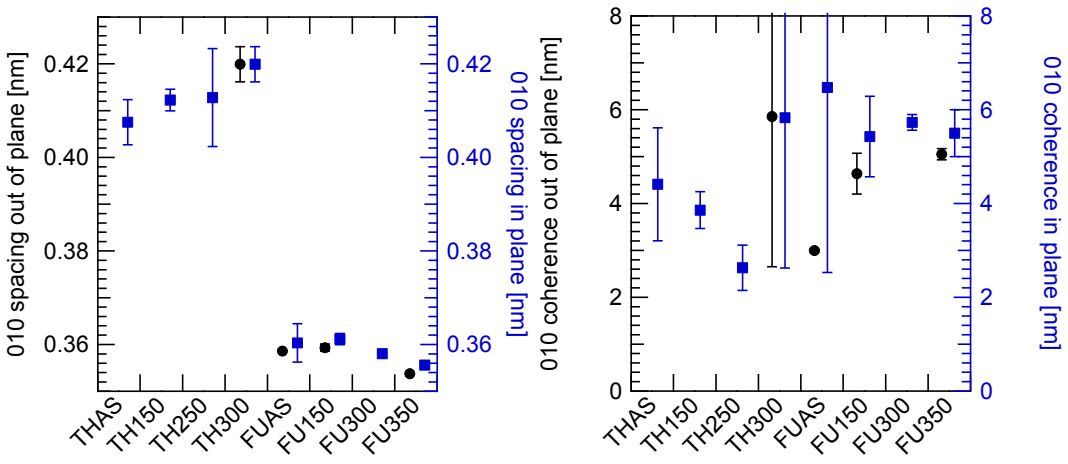


Figure S19. (010) π-πspacing, left, and (100) coherence length, right, as a function **4** (Fu) or **5b** (Th) and annealing temperature.

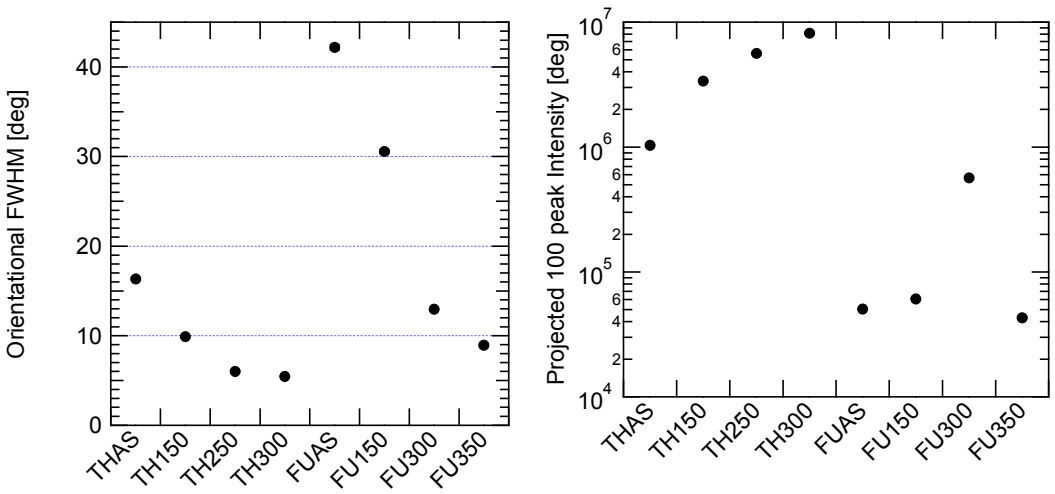


Figure S20. (100) orientational FWHM (measure of orientational disorder) and project (100) peak intensity as a function of **4** (Fu) or **5b** (Th) and annealing temperature.

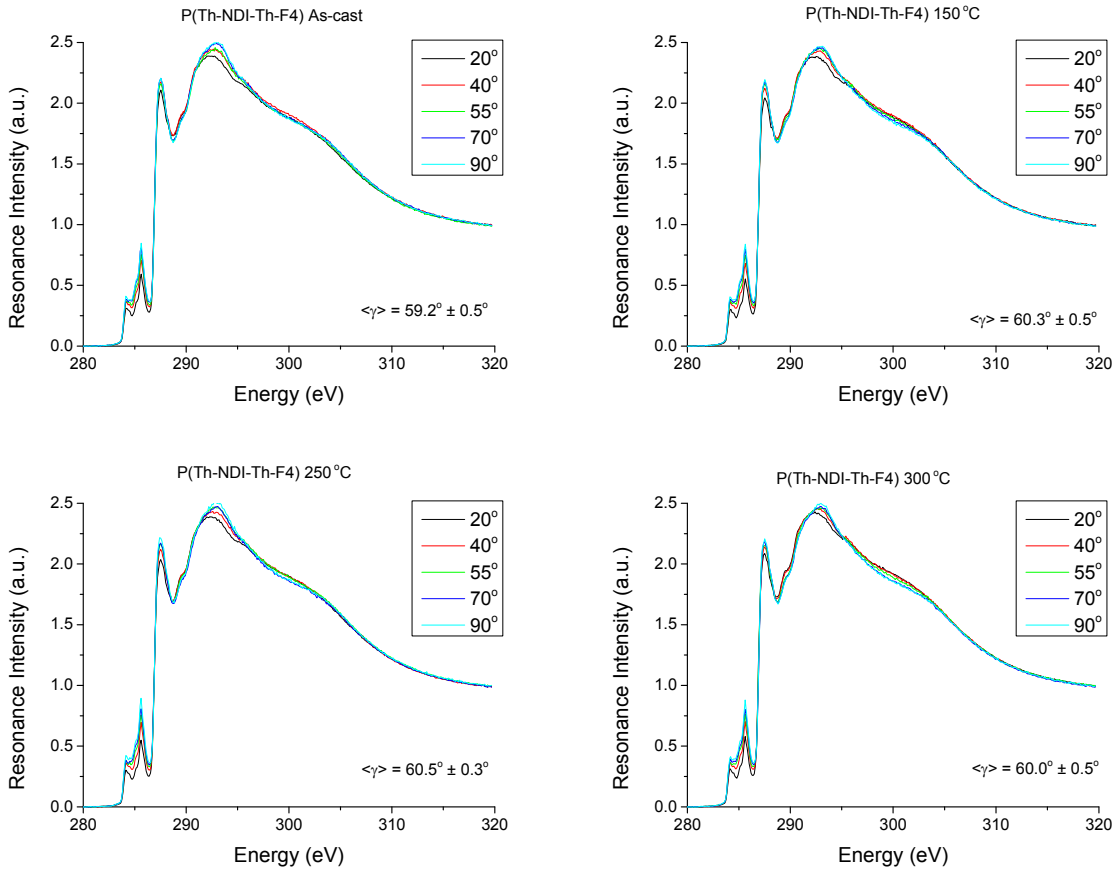


Figure S21. Full angle-resolved NEXAFS data set of P(ThNDIThF$_4$) **5b**.

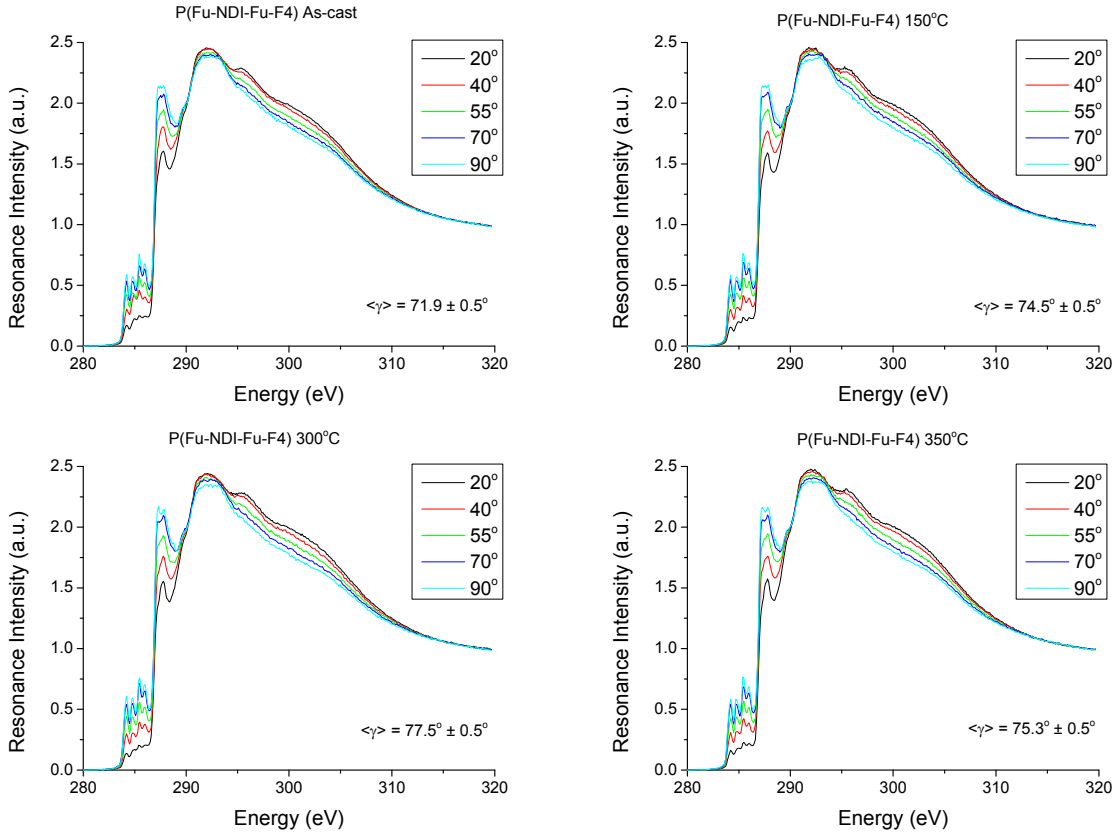


Figure S22. Full angle-resolved NEXAFS data set of P(FuNDIFuF$_4$) **4**.

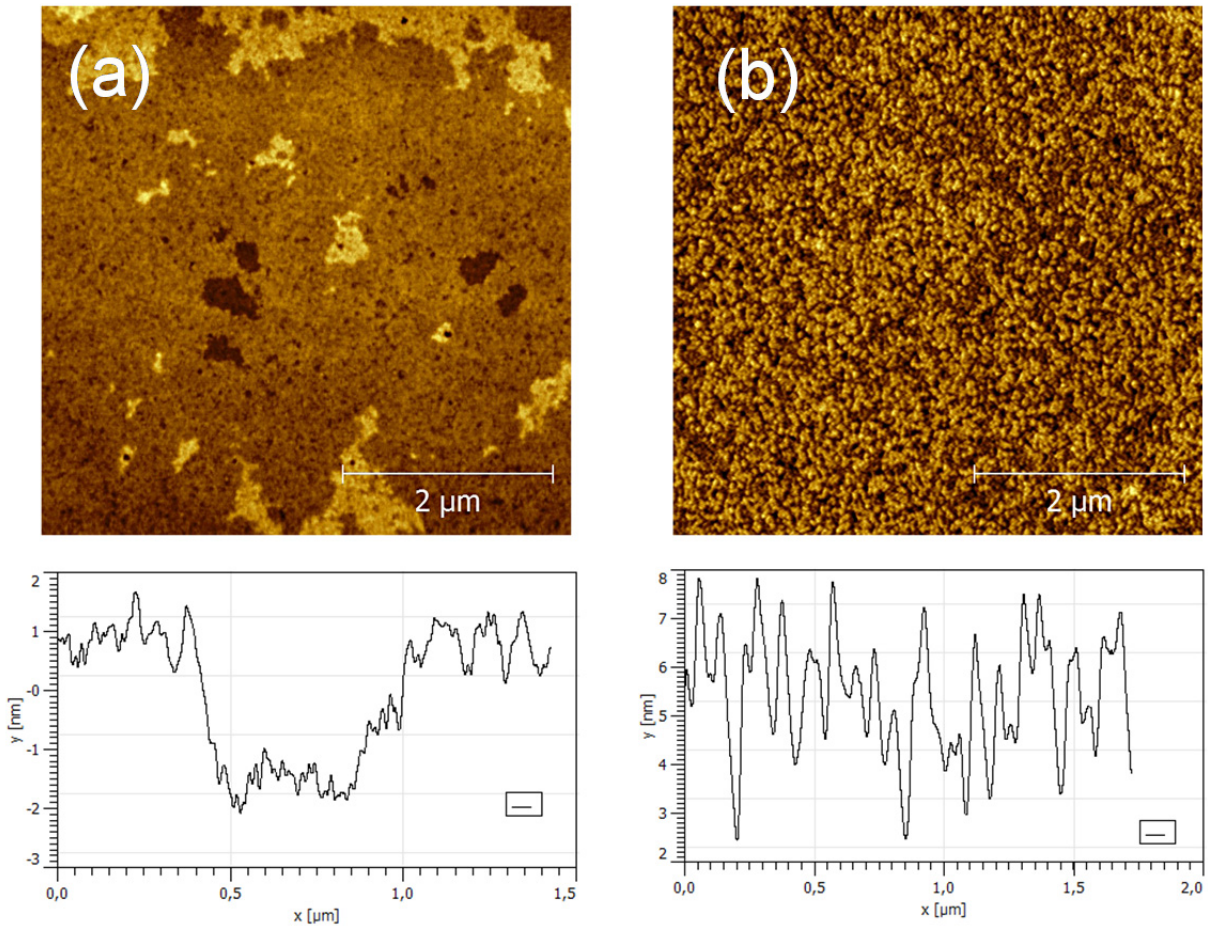


Figure S23. AFM images (phase mode) of films annealed at optimum OFET conditions a) P(ThNDIThF$_4$) **5b** and b) P(FuNDIFuF$_4$) **4**. Also shown are the height profiles with defined step heights corresponding to the (100) peak of P(ThNDIThF$_4$) in a), and the rough nodular morphology of P(FuNDIFuF$_4$) in b).

Optimized molecular structures at the B3LYP/6-31G level (atom number and Cartesian coordinates) of FuNDIFuF$_4$.**

7	-3.548979	3.686842	0.277161
6	-2.437633	2.840753	0.342407
6	-2.723688	1.386894	0.221348
6	-4.048040	0.910710	0.054898
6	-5.145272	1.811900	-0.009192
6	-4.878984	3.271508	0.112895
6	-6.451145	1.330209	-0.189111
6	-6.614840	-0.065134	-0.310613
6	-5.558740	-0.955263	-0.251308
6	-4.231448	-0.496508	-0.056316
6	-3.130723	-1.406988	0.020349
6	-3.423622	-2.852677	-0.162139
7	-4.754553	-3.245950	-0.376649
6	-5.859720	-2.395516	-0.413007
6	-1.818603	-0.905377	0.207867
6	-1.667076	0.513127	0.286462
6	-7.681816	2.197104	-0.267449
6	-0.566487	-1.647574	0.352808
8	0.554253	-0.865888	0.149655
6	1.659857	-1.608790	0.417398
6	1.269678	-2.873866	0.807639
6	-0.141286	-2.897630	0.761618
6	2.955224	-0.978470	0.243300
6	4.146977	-1.719048	0.340056
6	5.404616	-1.156714	0.181571
6	5.581382	0.213879	-0.092779
6	4.388042	0.954337	-0.186218
6	3.130536	0.393190	-0.024673
9	4.094296	-3.039446	0.594363
9	6.456472	-1.979479	0.297072
6	6.875111	0.845393	-0.270374
8	7.994815	0.053976	-0.169828
6	9.085959	0.844846	-0.370828
6	8.685268	2.132236	-0.598917
6	7.263299	2.139019	-0.535465
9	4.439487	2.275068	-0.439479
9	2.078469	1.217087	-0.127983
6	10.413055	0.177503	-0.304115
8	-2.568940	-3.729759	-0.147252
8	-1.306175	3.278096	0.491337
8	-5.760244	4.121107	0.075571
8	-6.995951	-2.820312	-0.575722
6	-4.977670	-4.686371	-0.554320
6	-3.333708	5.134685	0.390990
1	-7.606078	-0.479234	-0.461094
1	-4.405463	-5.045841	-1.411407
1	-4.640613	-5.226860	0.332382

1	-6.042609	-4.835019	-0.711592
1	-2.266839	5.299302	0.516201
1	-3.698196	5.634640	-0.508461
1	-3.887608	5.524853	1.246959
1	-0.679727	0.935765	0.412829
1	-0.776423	-3.731478	0.995227
1	1.920991	-3.684206	1.089034
1	-8.567597	1.573659	-0.411848
1	-7.808036	2.794817	0.638698
1	-7.612569	2.917144	-1.086653
1	6.609538	2.984583	-0.667931
1	9.332176	2.976158	-0.789878
1	11.205609	0.907651	-0.480477
1	10.578220	-0.282749	0.676479
1	10.498364	-0.614468	-1.056585

Optimized molecular structures at the ωB97XD/6-31G level (atom number and Cartesian coordinates) of FuNDIFuF$_4$.**

7	3.579688	3.673825	-0.232631
6	2.465788	2.846852	-0.352739
6	2.725469	1.388505	-0.235049
6	4.030255	0.894257	-0.009604
6	5.133247	1.778755	0.115032
6	4.890768	3.242449	-0.013824
6	6.412831	1.282385	0.353162
6	6.554591	-0.116689	0.472565
6	5.496665	-0.984116	0.352025
6	4.191509	-0.505206	0.094854
6	3.087510	-1.398003	-0.048718
6	3.351421	-2.853707	0.121233
7	4.656584	-3.263343	0.412725
6	5.765014	-2.431700	0.516520
6	1.807398	-0.882449	-0.290662
6	1.667498	0.533714	-0.362797
6	7.648237	2.129326	0.493382
6	0.553462	-1.614220	-0.504543
8	-0.555933	-0.860399	-0.239831
6	-1.647193	-1.565196	-0.603117
6	-1.263352	-2.775498	-1.113478
6	0.150760	-2.806185	-1.047870
6	-2.947546	-0.943409	-0.392049
6	-4.115681	-1.710069	-0.354005
6	-5.369825	-1.151653	-0.168811
6	-5.544613	0.226337	0.007063
6	-4.374471	0.992470	-0.032164
6	-3.121693	0.435871	-0.231955

9	-4.048416	-3.035791	-0.507616
9	-6.411517	-1.981711	-0.169531
6	-6.844665	0.849479	0.212611
8	-7.877502	0.043217	0.585717
6	-8.979734	0.817112	0.719208
6	-8.672145	2.112578	0.436683
6	-7.285734	2.138481	0.109987
9	-4.439938	2.318741	0.117395
9	-2.082307	1.268547	-0.273573
6	-10.231333	0.127252	1.124615
8	2.492766	-3.710576	0.030076
8	1.352791	3.295512	-0.544838
8	5.776618	4.074271	0.063637
8	6.878860	-2.869399	0.735390
6	4.849972	-4.702593	0.579898
6	3.390542	5.118621	-0.345853
1	7.532255	-0.544371	0.668437
1	4.210275	-5.068867	1.383630
1	4.580328	-5.222974	-0.340586
1	5.897480	-4.869246	0.815746
1	2.334292	5.301165	-0.523951
1	3.712412	5.607077	0.575112
1	3.991066	5.505824	-1.170171
1	0.689748	0.965165	-0.533974
1	0.793742	-3.609032	-1.358481
1	-1.916216	-3.546987	-1.486802
1	8.514556	1.494818	0.691959
1	7.831027	2.711640	-0.412168
1	7.542685	2.856604	1.300662
1	-6.693901	2.994359	-0.169341
1	-9.355329	2.948269	0.459458
1	-11.042097	0.853323	1.203369
1	-10.515532	-0.634321	0.392386
1	-10.111610	-0.367418	2.093157

Optimized molecular structures at the LC-BLYP/6-31G (μ = 0.2 a_0^{-1}) level (atom number and Cartesian coordinates) of $FuNDIFuF_4$.**

7	3.321544	3.694646	-0.100335
6	2.249022	2.797356	-0.122727
6	2.612386	1.358261	-0.080706
6	3.965971	0.945719	-0.021358
6	5.019231	1.898877	0.001566
6	4.677155	3.343406	-0.042259
6	6.353884	1.485380	0.065811
6	6.598305	0.095707	0.109750
6	5.584206	-0.840332	0.088116
6	4.224039	-0.446748	0.017747
6	3.163053	-1.409397	-0.010004

6	3.545797	-2.840593	0.053558
7	4.907048	-3.170450	0.133507
6	5.968892	-2.266556	0.147519
6	1.821568	-0.973784	-0.075850
6	1.596525	0.439728	-0.104807
6	7.525979	2.422964	0.092930
6	0.588882	-1.766949	-0.124201
8	-0.535276	-0.965366	-0.039125
6	-1.636489	-1.748714	-0.142704
6	-1.254285	-3.062243	-0.295629
6	0.162843	-3.073722	-0.282348
6	-2.923867	-1.080270	-0.077425
6	-4.116826	-1.815882	-0.098861
6	-5.369940	-1.218983	-0.043788
6	-5.517931	0.175139	0.037454
6	-4.322979	0.910127	0.058004
6	-3.069309	0.314238	0.001506
9	-4.070964	-3.158093	-0.175134
9	-6.438036	-2.026740	-0.069863
6	-6.803556	0.845635	0.096828
8	-7.930825	0.061369	0.059320
6	-9.011338	0.893232	0.126498
6	-8.591338	2.193127	0.206057
6	-7.166136	2.168251	0.187134
9	-4.364883	2.252418	0.131461
9	-2.003290	1.127250	0.021835
6	-10.344516	0.242547	0.100393
8	2.742589	-3.771123	0.045248
8	1.087170	3.185544	-0.174588
8	5.518876	4.239576	-0.029693
8	7.136435	-2.640780	0.207921
6	5.214625	-4.597473	0.196077
6	3.030113	5.125397	-0.141189
1	7.623662	-0.281682	0.164794
1	4.732388	-5.044079	1.076759
1	4.824208	-5.102945	-0.698314
1	6.305021	-4.686936	0.254702
1	1.940538	5.230467	-0.188774
1	3.435166	5.613793	0.756259

Optimized molecular structures at the B3LYP/6-31G level (atom number and Cartesian coordinates) of $ThNDIThF_4$.**

16	-8.567551	-0.587078	0.307614
6	-7.257977	0.102435	-0.656220
6	-7.793180	0.818349	-1.711179
6	-9.211327	0.814133	-1.744473
6	-9.787238	0.102527	-0.723896
6	-5.850855	-0.095119	-0.316934
6	-4.795301	0.495880	-1.038343
6	-3.460313	0.307928	-0.714187
6	-3.023350	-0.484664	0.362612
6	-4.077844	-1.074442	1.085552
6	-5.413093	-0.888589	0.759603
6	-1.614923	-0.676619	0.704336
16	-0.325520	0.181667	-0.128313
6	0.899981	-0.576374	0.847068
6	0.334677	-1.459856	1.739089
6	-1.077002	-1.503182	1.676929
6	2.342791	-0.402891	0.589991
6	3.067704	-1.593495	0.326195
6	4.405285	-1.588226	-0.010593
6	5.109775	-0.365457	-0.130911
6	4.407045	0.837815	0.157473
6	3.037476	0.816854	0.544250
6	6.478347	-0.339879	-0.520307
6	7.163292	-1.632265	-0.796216
7	6.420399	-2.814608	-0.647991
6	5.075245	-2.887463	-0.273128
6	7.158230	0.880990	-0.638060
6	6.438470	2.064677	-0.351726
6	5.114316	2.059256	0.037731
6	4.453484	3.357934	0.325796
7	3.137052	3.281898	0.788087
6	2.415303	2.095366	1.000432
6	8.602723	1.016708	-1.046379
8	1.330030	2.154388	1.556271
6	2.461768	4.525421	1.181248
8	5.026668	4.429203	0.187001
8	4.492836	-3.957442	-0.168555
6	7.138359	-4.065880	-0.922636
8	8.335603	-1.712589	-1.140235
9	-2.557576	0.935325	-1.492624
9	-5.044073	1.286926	-2.098883
9	-6.314400	-1.514008	1.541198
9	-3.828510	-1.858214	2.150832
6	-11.244781	-0.113363	-0.448390
1	6.932916	3.026593	-0.435525
1	1.479074	4.568548	0.710080
1	2.324049	4.552264	2.264695

1	3.085422	5.355050	0.858886
1	6.446334	-4.886301	-0.752447
1	7.493870	-4.070336	-1.954887
1	8.003896	-4.146826	-0.262579
1	2.554623	-2.547503	0.362563
1	0.920386	-2.046111	2.437930
1	-1.678009	-2.125046	2.321830
1	-7.187744	1.331904	-2.442093
1	-9.791216	1.325426	-2.505183
1	-11.843694	0.393547	-1.209533
1	-11.510159	-1.176365	-0.463672
1	-11.538156	0.283002	0.530146
1	9.262425	0.474208	-0.364546
1	8.780914	0.582804	-2.033504
1	8.889471	2.070890	-1.060595

Optimized molecular structures at the ωB97XD/6-31G level (atom number and Cartesian coordinates) of ThNDIThF$_4$.**

16	-8.520764	-0.532241	0.351425
6	-7.219712	0.006174	-0.679772
6	-7.727482	0.562180	-1.826545
6	-9.146475	0.555553	-1.874398
6	-9.724980	0.006377	-0.766392
6	-5.810101	-0.115219	-0.295484
6	-4.821236	0.726159	-0.817798
6	-3.486228	0.612462	-0.465401
6	-3.019094	-0.343681	0.441272
6	-4.007536	-1.185212	0.963804
6	-5.342564	-1.071928	0.610550
6	-1.608284	-0.462896	0.824947
16	-0.318763	0.092123	-0.204685
6	0.883259	-0.448505	0.909023
6	0.318821	-1.034904	2.005759
6	-1.098062	-1.034863	1.964187
6	2.325535	-0.348238	0.597368
6	2.995961	-1.566376	0.337826
6	4.323860	-1.605659	-0.008659
6	5.065896	-0.411014	-0.142253
6	4.410818	0.810556	0.128754
6	3.047090	0.838033	0.519288
6	6.431604	-0.434011	-0.534936
6	7.071549	-1.752157	-0.798255
7	6.295545	-2.902833	-0.626288
6	4.953291	-2.927257	-0.256509
6	7.145431	0.753642	-0.669187
6	6.466423	1.966222	-0.399746
6	5.151670	2.005615	-0.011984
6	4.524243	3.327766	0.246829

7	3.202999	3.301387	0.683432
6	2.446072	2.147691	0.915194
6	8.589496	0.836875	-1.082148
8	1.351571	2.250217	1.428876
6	2.555850	4.568240	1.019851
8	5.130318	4.371298	0.098048
8	4.338045	-3.969704	-0.142885
6	6.967002	-4.175286	-0.884568
8	8.230871	-1.872606	-1.149958
9	-2.630827	1.469561	-1.032423
9	-5.137716	1.694073	-1.683193
9	-6.197018	-1.931835	1.174643
9	-3.690907	-2.154084	1.827954
6	-11.183216	-0.172139	-0.476289
1	6.991132	2.910409	-0.501571
1	1.588310	4.624826	0.520850
1	2.393877	4.633166	2.097504
1	3.209136	5.371284	0.689206
1	6.280785	-4.972052	-0.610320
1	7.230316	-4.251832	-1.941247
1	7.882444	-4.230754	-0.295198
1	2.448904	-2.500323	0.403891
1	0.900431	-1.434417	2.827329
1	-1.717787	-1.441980	2.749270
1	-7.104345	0.961045	-2.613857
1	-9.721193	0.945659	-2.706148
1	-11.773117	0.214858	-1.310140
1	-11.440137	-1.226969	-0.339570
1	-11.483707	0.364123	0.429068
1	9.229703	0.281988	-0.393402
1	8.745285	0.384719	-2.063695
1	8.910955	1.879971	-1.111277

Optimized molecular structures at the LC-BLYP/6-31G (μ = 0.2 a_0^{-1}) level (atom number and Cartesian coordinates) of $ThNDIThF_4$.**

16	-8.531992	-0.761661	0.200758
6	-7.260086	0.157819	-0.586781
6	-7.808268	1.043532	-1.493497
6	-9.225469	0.981886	-1.552090
6	-9.770383	0.056431	-0.698352
6	-5.848760	-0.046004	-0.270491
6	-4.816682	0.675399	-0.891562
6	-3.476664	0.476717	-0.586064
6	-3.031892	-0.454203	0.363605
6	-4.063134	-1.175622	0.985319
6	-5.403278	-0.977463	0.679005
6	-1.618443	-0.659906	0.676166
16	-0.362493	0.302550	-0.066686

6	0.880046	-0.541818	0.798576
6	0.340005	-1.519876	1.607105
6	-1.072324	-1.575814	1.557854
6	2.321929	-0.373351	0.535490
6	3.030446	-1.576741	0.273783
6	4.370276	-1.590500	-0.040602
6	5.100073	-0.381061	-0.135644
6	4.416936	0.828516	0.143836
6	3.036675	0.831010	0.496146
6	6.476701	-0.379151	-0.494343
6	7.142204	-1.677527	-0.769040
7	6.372979	-2.844840	-0.652005
6	5.019763	-2.897862	-0.303989
6	7.186245	0.821887	-0.584396
6	6.487388	2.019972	-0.300232
6	5.155939	2.034428	0.054862
6	4.521294	3.342323	0.346622
7	3.186906	3.289805	0.756089
6	2.419380	2.124339	0.905023
6	8.636919	0.912287	-0.959149
8	1.290136	2.221411	1.371697
6	2.526120	4.538946	1.128272
8	5.126785	4.405165	0.252575
8	4.415703	-3.962403	-0.223530
6	7.068013	-4.100425	-0.925950
8	8.324743	-1.779674	-1.088885
9	-2.581764	1.231130	-1.251938
9	-5.088333	1.604026	-1.826672
9	-6.296942	-1.733651	1.344871
9	-3.791503	-2.103691	1.920610
6	-11.214307	-0.276583	-0.495739
1	7.003294	2.983035	-0.356548
1	1.600364	4.652821	0.547713
1	2.258613	4.518012	2.194354
1	3.230264	5.351361	0.917336
1	6.342505	-4.908615	-0.781384
1	7.453283	-4.096260	-1.955322

Optimized molecular structures at the LC-BLYP/6-31G (μ = 0.2 a_0^{-1}) level (atom number and Cartesian coordinates) for tetramer of $FuNDIFuF_4$.**

C	31.945059	2.641061	-1.185983
C	31.698245	1.295085	-1.057990
O	32.889319	0.612667	-1.001154
C	33.893751	1.532715	-1.093666
C	33.362796	2.788623	-1.208442
C	30.475480	0.517663	-0.977047
C	30.448661	-0.880759	-0.851587
C	29.252272	-1.582511	-0.776856
C	27.999848	-0.954757	-0.821011
C	28.023858	0.443444	-0.950003
C	29.221071	1.144477	-1.022471
C	26.775465	-1.731311	-0.743622
O	25.611588	-1.036715	-0.717593
C	24.561728	-1.934088	-0.643258
C	25.097855	-3.209167	-0.622548
C	26.507681	-3.080486	-0.688270
C	23.265416	-1.249959	-0.677788
C	23.357419	0.148109	-0.950554
C	22.263580	0.969370	-1.046448
C	20.947086	0.470799	-0.874274
C	20.830328	-0.910998	-0.580855
C	21.968306	-1.772537	-0.483895
C	19.516229	-1.402890	-0.378199
C	18.421565	-0.582349	-0.480009
C	18.511956	0.805666	-0.794241
C	19.808736	1.328957	-0.985502
C	22.519887	2.399030	-1.334393
N	21.381916	3.200927	-1.419103
C	20.059036	2.762903	-1.276254
C	21.719945	-3.197098	-0.152343
N	20.400239	-3.621997	0.053446
C	19.262200	-2.822936	-0.044594
C	17.212467	1.483562	-0.870959
C	16.650865	2.667703	-1.312280
C	15.248403	2.567068	-1.132758
C	15.012203	1.325932	-0.586777
O	16.188114	0.668960	-0.427275
C	13.809569	0.625373	-0.174235
C	13.806572	-0.705214	0.276248
C	12.629329	-1.336731	0.657295
C	11.380372	-0.700560	0.615801
C	11.383383	0.630087	0.165693
C	12.560591	1.261612	-0.215464
C	10.177779	-1.401946	1.027215
O	9.001147	-0.746835	0.865927
C	7.977471	-1.563868	1.307307
C	8.540504	-2.747144	1.749332

C	9.942886	-2.643743	1.572574
C	6.677213	-0.888881	1.231110
C	6.765157	0.502173	0.927035
C	5.668961	1.320790	0.829759
C	4.355653	0.823559	1.025864
C	4.241009	-0.561285	1.305606
C	5.381434	-1.417386	1.413742
C	2.925590	-1.065431	1.466114
C	1.829693	-0.245986	1.372924
C	1.920472	1.154253	1.116384
C	3.216184	1.682820	0.934344
C	5.919062	2.744192	0.506912
N	4.778678	3.541395	0.413859
C	3.460746	3.112272	0.618198
C	5.134000	-2.854433	1.690714
N	3.811299	-3.297992	1.820997
C	2.671849	-2.498733	1.738076
O	1.545266	-2.962328	1.880303
C	3.637927	-4.724625	2.084938
O	6.024100	-3.693624	1.808473
O	2.571019	3.953953	0.515999
C	4.948775	4.957645	0.097111
O	7.043284	3.201294	0.329861
F	12.714912	-2.610572	1.075784
F	14.937403	-1.419706	0.351258
F	12.475069	2.535426	-0.634102
F	10.252152	1.344238	0.091020
O	23.646528	2.858678	-1.487545
C	21.558191	4.624374	-1.697462
O	19.170692	3.603917	-1.395418
O	22.606669	-4.040530	-0.038342
C	20.227037	-5.034834	0.382935
O	18.136595	-3.275540	0.136889
F	29.323749	-2.920472	-0.657784
F	31.582527	-1.591501	-0.798102
F	29.145901	2.481795	-1.144066
F	26.891244	1.158183	-1.011280
C	35.278161	1.000623	-1.052105
C	0.622217	1.837158	1.082347
O	-0.425413	0.936250	1.103655
C	-1.591248	1.628333	1.142508
C	-1.325143	2.978819	1.148418
C	0.085549	3.111447	1.107985
C	-2.814476	0.846981	1.169058
C	-2.833488	-0.555416	1.249179
C	-4.029239	-1.262106	1.271470
C	-5.281832	-0.633797	1.221748
C	-5.263015	0.769022	1.150861
C	-4.067144	1.475531	1.123238
F	-1.700041	-1.267274	1.308699
F	-3.957957	-2.601547	1.347086

C	-6.504321	-1.416042	1.252519
O	-7.669520	-0.738307	1.100073
C	-8.714403	-1.641279	1.153573
C	-8.176984	-2.901134	1.343242
C	-6.768527	-2.757887	1.408398
F	-6.397353	1.480773	1.109053
F	-4.137858	2.815329	1.053450
C	-10.015273	-0.968023	1.073951
C	-11.301928	-1.523645	0.909077
C	-12.447785	-0.668868	0.874444
C	-12.348783	0.738739	1.008650
C	-11.041382	1.267981	1.154449
C	-9.939012	0.452230	1.182615
C	-13.751873	-1.194948	0.693253
C	-13.984970	-2.646326	0.514250
N	-12.838318	-3.439259	0.538514
C	-11.529403	-2.980307	0.736559
C	-14.854867	-0.380123	0.672713
C	-14.783736	1.035797	0.831253
C	-13.496547	1.591833	0.991644
C	-13.264914	3.052457	1.118079
N	-11.949456	3.518193	1.242632
C	-10.803822	2.724161	1.280593
C	-16.090345	1.702883	0.804493
O	-17.098337	0.830478	0.440357
C	-18.283378	1.487135	0.503198
C	-18.069611	2.785610	0.906855
C	-16.671750	2.923247	1.096659
O	-9.684806	3.209833	1.407628
C	-11.791607	4.966357	1.356410
O	-14.162422	3.892081	1.113762
O	-10.632902	-3.820871	0.748957
C	-12.991161	-4.882160	0.366041
O	-15.101106	-3.128639	0.353285
C	-19.470784	0.728851	0.153165
C	-19.448761	-0.640861	-0.158183
C	-20.611556	-1.326710	-0.485895
C	-21.870139	-0.709647	-0.523493
C	-21.893248	0.658185	-0.204478
C	-20.729818	1.345287	0.118338
F	-18.306406	-1.340754	-0.150273
F	-20.501633	-2.634742	-0.772033
C	-23.058420	-1.470071	-0.865995
O	-24.221377	-0.778495	-0.961020
C	-25.232916	-1.660106	-1.292138
C	-24.676254	-2.921131	-1.403329
C	-23.290844	-2.800879	-1.129625
F	-23.038261	1.353891	-0.196877
F	-20.840365	2.652176	0.409597
C	-26.538559	-0.992133	-1.340223
C	-27.775935	-1.488220	-1.803096

C	-28.941327	-0.657605	-1.746518
C	-28.890287	0.659964	-1.228429
C	-27.635907	1.137614	-0.777015
C	-26.518670	0.346485	-0.835953
C	-30.201746	-1.112534	-2.209723
C	-30.365411	-2.463333	-2.788183
N	-29.203565	-3.233531	-2.841447
C	-27.936864	-2.844783	-2.382112
C	-31.319399	-0.305733	-2.144332
C	-31.283223	1.005832	-1.622279
C	-30.049057	1.479966	-1.166190
C	-29.924791	2.851553	-0.610169
N	-28.659270	3.271876	-0.178094
C	-27.489640	2.506883	-0.221633
O	-31.441588	-2.887118	-3.198659
C	-29.292323	-4.578581	-3.405562
O	-27.023339	-3.659582	-2.493202
C	-32.554799	1.803019	-1.592639
O	-30.870755	3.630619	-0.512023
C	-28.582137	4.627946	0.359607
O	-26.417221	2.947858	0.176923
H	17.446471	-1.040474	-0.306304
H	20.633168	-5.658992	-0.425359
H	20.776144	-5.272204	1.304758
H	19.151868	-5.203857	0.508895
H	22.635975	4.801895	-1.782793
H	21.039019	4.889388	-2.629180
H	21.121752	5.219747	-0.883432
H	24.334625	0.612201	-1.094074
H	24.526885	-4.125231	-0.563379
H	27.243832	-3.877731	-0.693111
H	31.192383	3.419607	-1.254614
H	33.927093	3.713868	-1.298856
H	0.852981	-0.714431	1.505177
H	4.081922	-5.310813	1.268364
H	4.151666	-4.996552	3.017661
H	2.560237	-4.906653	2.161318
H	6.023284	5.129675	-0.030286
H	4.396622	5.202519	-0.820886
H	4.544132	5.573619	0.912411
H	7.739870	0.963100	0.758290
H	7.992223	-3.588414	2.149969
H	10.695124	-3.388045	1.812912
H	14.497181	3.312757	-1.372099
H	17.200133	3.507664	-1.714254
H	35.996815	1.827792	-1.131825
H	35.471383	0.461221	-0.110958
H	35.462287	0.298643	-1.881205
H	-15.821359	-0.865178	0.526103
H	-12.409060	-5.216472	-0.503956
H	-12.609213	-5.406565	1.253169

H	-14.060239	-5.075456	0.224341
H	-10.718068	5.164381	1.449571
H	-12.209189	5.457333	0.466382
H	-12.339004	5.333134	2.235962
H	-8.968867	0.939519	1.294267
H	-8.745449	-3.817515	1.420806
H	-6.031345	-3.541498	1.550315
H	-2.062206	3.774834	1.176696
H	0.656148	4.029709	1.094959
H	-32.258265	-0.722642	-2.520564
H	-28.608917	-4.669061	-4.261301
H	-28.993293	-5.320058	-2.651459
H	-30.333112	-4.728091	-3.713409
H	-27.539558	4.800866	0.648719
H	-28.905343	5.349801	-0.403520
H	-29.253316	4.724045	1.224581
H	-25.583589	0.778717	-0.475840
H	-25.217071	-3.822016	-1.657892
H	-22.547685	-3.591652	-1.126595
H	-18.832463	3.544794	1.045984
H	-16.138249	3.810631	1.407852
H	-32.451008	2.740626	-2.158385
H	-33.381041	1.208820	-2.009286
H	-32.804694	2.116885	-0.568425

Optimized molecular structures at the LC-BLYP/6-31G (μ = 0.2 a_0^{-1}) level (atom number and Cartesian coordinates) for tetramer of ThNDIThF$_4$.**

C	-31.715223	2.726727	-0.584950
C	-31.514563	1.257546	-0.523760
C	-32.593116	0.361591	-0.711881
C	-33.904765	0.843919	-0.977552
C	-34.126810	2.310796	-1.042115
N	-33.021236	3.150624	-0.844480
C	-30.250625	0.785071	-0.266539
C	-29.949852	-0.602953	-0.165433
C	-31.005110	-1.514085	-0.356062
C	-32.319434	-1.027394	-0.634010
C	-33.405875	-1.910819	-0.857678
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N	-31.911097	-3.812414	-0.603693
C	-30.802994	-2.992010	-0.335442
C	-34.671287	-1.428923	-1.116209
C	-34.963160	-0.046415	-1.178170
C	-28.541144	-0.921273	0.132797
S	-27.307778	0.062839	-0.616770
C	-26.036801	-0.736655	0.272747
C	-26.571192	-1.700298	1.111206
C	-27.976961	-1.805692	1.026128
C	-24.629258	-0.393634	0.084383
C	-23.587266	-1.061203	0.747861

C	-22.252372	-0.723782	0.567353
C	-21.825381	0.306548	-0.283349
C	-22.867345	0.973445	-0.947559
C	-24.202218	0.636110	-0.767010
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C	-18.479775	1.739003	-1.201267
C	-19.886993	1.646685	-1.273186
C	-16.501365	0.466549	-0.096629
C	-16.209347	-0.924811	-0.069713
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C	-13.847949	-0.555039	0.360864
C	-14.117238	0.838743	0.341107
C	-15.430270	1.353429	0.113632
C	-13.019562	1.706399	0.562767
C	-11.756050	1.209116	0.769418
C	-11.461232	-0.182232	0.787806
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C	-13.192084	3.177308	0.612812
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C	-4.403176	1.438848	-0.097556
C	-5.733473	1.104219	0.118427
C	-1.939498	1.021281	0.196308
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C	-0.018369	2.166479	-0.491235
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C	2.221578	-0.705566	0.015076
C	3.475104	-1.266494	0.048514
C	4.618800	-0.479638	0.330761
C	4.404199	0.904593	0.561711
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C	5.923141	-1.061367	0.372830
C	7.040164	-0.252395	0.649812
C	6.800540	1.130302	0.881697
C	5.547222	1.691171	0.847398

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C	6.048111	-2.515487	0.062103
C	8.450855	-0.670792	0.737061
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C	10.457807	-1.705492	1.326362
C	9.046704	-1.750436	1.352484
C	12.365217	-0.255193	0.436884
C	13.425725	-1.093549	0.816191
C	14.754755	-0.763331	0.586177
C	15.157180	0.427527	-0.036521
C	14.096424	1.265455	-0.416554
C	12.767401	0.935343	-0.186371
C	16.558276	0.763524	-0.278172
C	17.066776	1.900012	-0.884190
C	18.477891	1.933194	-0.927907
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S	17.858496	-0.287339	0.222892
C	20.478601	0.385518	-0.323553
C	20.701077	-0.983766	-0.634883
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C	23.103958	-0.798393	-0.334641
C	22.905217	0.572003	-0.021447
C	21.606753	1.167216	-0.016098
C	24.403028	-1.393712	-0.340256
C	25.531362	-0.612497	-0.030219
C	25.307290	0.757408	0.281547
C	24.059369	1.330611	0.294415
C	21.499206	2.603879	0.372682
N	22.677266	3.285794	0.716056
C	23.966428	2.757109	0.684072
C	22.041804	-2.983068	-1.039661
N	23.330753	-3.510709	-1.075895
C	24.509942	-2.828605	-0.734606
C	26.938260	-1.047509	0.019915
S	28.155810	0.074055	-0.541814
C	29.452655	-0.983817	-0.048482
C	28.940740	-2.130980	0.533669
C	27.529335	-2.166960	0.564891
C	30.855392	-0.642474	-0.274822
C	31.913013	-1.500853	0.064791
C	33.243900	-1.164531	-0.146205
C	33.652703	0.051976	-0.712917
C	32.593821	0.908978	-1.053934
C	31.263230	0.573893	-0.841320
C	35.054406	0.398402	-0.931588
C	35.567554	1.558860	-1.476994

C	36.985509	1.568337	-1.544291
C	37.565859	0.425294	-1.055217
S	36.360825	-0.692105	-0.498433
C	39.021229	0.091512	-0.969620
F	34.165751	-2.074056	0.222752
F	31.676785	-2.704408	0.616660
F	30.339025	1.480380	-1.211733
F	32.829244	2.112151	-1.607790
O	24.951384	3.431153	0.967251
C	22.512979	4.686144	1.100476
O	20.445005	3.228901	0.417644
O	25.563865	-3.453443	-0.786883
C	23.495001	-4.909954	-1.464302
O	21.055857	-3.656997	-1.320325
F	15.682077	-1.649004	0.994957
F	13.194309	-2.270106	1.423795
F	11.839551	1.818938	-0.598537
F	14.327343	2.441057	-1.026288
O	6.411697	3.834901	1.410407
C	3.960688	5.072738	1.439259
O	1.915036	3.559049	0.812187
O	7.109132	-3.130362	0.054328
C	5.060640	-4.646290	-0.552988
O	2.608268	-3.411752	-0.504867
F	-2.816670	-1.242026	1.718535
F	-5.307607	-1.871018	2.122478
F	-6.661882	1.903106	-0.439382
F	-4.171209	2.535606	-0.839431
O	-15.711832	-3.662516	-0.095657
C	-13.229268	-4.790245	0.228805
O	-11.271733	-3.114843	0.699871
O	-16.693522	3.397429	-0.007682
C	-14.738541	5.073795	0.476162
O	-12.256837	3.946356	0.809359
F	-21.344529	-1.437336	1.259040
F	-23.842739	-2.072201	1.596190
F	-25.109573	1.347080	-1.461837
F	-22.611946	1.982999	-1.797695
O	-34.135574	-4.168314	-1.032089
C	-31.654505	-5.250996	-0.583181
O	-29.730362	-3.540377	-0.104993
C	-36.375503	0.375607	-1.460827
O	-35.223826	2.820972	-1.259369
C	-33.283861	4.585974	-0.917586
O	-30.798352	3.524241	-0.419376
H	19.860870	-1.627206	-0.909490
H	24.158881	-4.976972	-2.337226
H	23.957385	-5.473505	-0.641748
H	22.496955	-5.298589	-1.694760
H	23.510457	5.074127	1.334459
H	22.055000	5.248390	0.274558

H	21.845349	4.755932	1.970315
H	26.146986	1.400606	0.558240
H	26.957866	-2.998862	0.968690
H	29.573652	-2.925318	0.921017
H	34.936764	2.376423	-1.817092
H	37.568690	2.399656	-1.944618
H	1.390226	-1.371820	-0.230530
H	5.731107	-4.757173	-1.416359
H	5.523176	-5.155542	0.304134
H	4.068357	-5.058567	-0.766595
H	4.951409	5.483156	1.663443
H	3.509034	5.582034	0.576351
H	3.280776	5.186092	2.294870
H	7.630985	1.796330	1.131022
H	8.478987	-2.561188	1.802048
H	11.094010	-2.470458	1.764225
H	16.432319	2.689319	-1.279203
H	19.047857	2.757792	-1.348677
H	39.615130	0.925413	-1.371553
H	39.342191	-0.083136	0.069887
H	39.270188	-0.812108	-1.548930
H	-17.001987	-1.654937	-0.254343
H	-12.501148	-5.019475	-0.561520
H	-12.808784	-5.127746	1.186465
H	-14.193213	-5.271533	0.030375
H	-13.775895	5.555180	0.680573
H	-15.154268	5.413192	-0.482912
H	-15.470855	5.300917	1.263216
H	-10.964046	1.939854	0.954263
H	-10.025414	-2.210990	2.388268
H	-7.416108	-2.025330	2.475868
H	-2.063648	2.877210	-0.929269
H	0.552412	2.968645	-0.952483
H	-35.463117	-2.165694	-1.280697
H	-30.893794	-5.503048	-1.334935
H	-31.268546	-5.546855	0.402454
H	-32.605501	-5.749962	-0.799571
H	-32.329124	5.097181	-0.751676
H	-33.701351	4.837273	-1.902582
H	-34.021007	4.869114	-0.153137
H	-29.464220	1.528462	-0.110516
H	-28.562791	-2.521442	1.597428
H	-25.958270	-2.315943	1.764604
H	-20.503458	2.295381	-1.890198
H	-17.896189	2.476075	-1.747332
H	-36.432088	0.998882	-2.365513
H	-37.016319	-0.509898	-1.581002
H	-36.770220	1.011384	-0.654614

Optimized molecular structures at the B3LYP/6-31G level (atom number and Cartesian coordinates) for tetramer of FuNDIFuF$_4$.**

C	31.945059	2.641061	-1.185983
C	31.698245	1.295085	-1.057990
O	32.889319	0.612667	-1.001154
C	33.893751	1.532715	-1.093666
C	33.362796	2.788623	-1.208442
C	30.475480	0.517663	-0.977047
C	30.448661	-0.880759	-0.851587
C	29.252272	-1.582511	-0.776856
C	27.999848	-0.954757	-0.821011
C	28.023858	0.443444	-0.950003
C	29.221071	1.144477	-1.022471
C	26.775465	-1.731311	-0.743622
O	25.611588	-1.036715	-0.717593
C	24.561728	-1.934088	-0.643258
C	25.097855	-3.209167	-0.622548
C	26.507681	-3.080486	-0.688270
C	23.265416	-1.249959	-0.677788
C	23.357419	0.148109	-0.950554
C	22.263580	0.969370	-1.046448
C	20.947086	0.470799	-0.874274
C	20.830328	-0.910998	-0.580855
C	21.968306	-1.772537	-0.483895
C	19.516229	-1.402890	-0.378199
C	18.421565	-0.582349	-0.480009
C	18.511956	0.805666	-0.794241
C	19.808736	1.328957	-0.985502
C	22.519887	2.399030	-1.334393
N	21.381916	3.200927	-1.419103
C	20.059036	2.762903	-1.276254
C	21.719945	-3.197098	-0.152343
N	20.400239	-3.621997	0.053446
C	19.262200	-2.822936	-0.044594
C	17.212467	1.483562	-0.870959
C	16.650865	2.667703	-1.312280
C	15.248403	2.567068	-1.132758
C	15.012203	1.325932	-0.586777
O	16.188114	0.668960	-0.427275
C	13.809569	0.625373	-0.174235
C	13.806572	-0.705214	0.276248
C	12.629329	-1.336731	0.657295
C	11.380372	-0.700560	0.615801
C	11.383383	0.630087	0.165693
C	12.560591	1.261612	-0.215464
C	10.177779	-1.401946	1.027215
O	9.001147	-0.746835	0.865927
C	7.977471	-1.563868	1.307307
C	8.540504	-2.747144	1.749332
C	9.942886	-2.643743	1.572574

C	6.677213	-0.888881	1.231110
C	6.765157	0.502173	0.927035
C	5.668961	1.320790	0.829759
C	4.355653	0.823559	1.025864
C	4.241009	-0.561285	1.305606
C	5.381434	-1.417386	1.413742
C	2.925590	-1.065431	1.466114
C	1.829693	-0.245986	1.372924
C	1.920472	1.154253	1.116384
C	3.216184	1.682820	0.934344
C	5.919062	2.744192	0.506912
N	4.778678	3.541395	0.413859
C	3.460746	3.112272	0.618198
C	5.134000	-2.854433	1.690714
N	3.811299	-3.297992	1.820997
C	2.671849	-2.498733	1.738076
O	1.545266	-2.962328	1.880303
C	3.637927	-4.724625	2.084938
O	6.024100	-3.693624	1.808473
O	2.571019	3.953953	0.515999
C	4.948775	4.957645	0.097111
O	7.043284	3.201294	0.329861
F	12.714912	-2.610572	1.075784
F	14.937403	-1.419706	0.351258
F	12.475069	2.535426	-0.634102
F	10.252152	1.344238	0.091020
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C	21.558191	4.624374	-1.697462
O	19.170692	3.603917	-1.395418
O	22.606669	-4.040530	-0.038342
C	20.227037	-5.034834	0.382935
O	18.136595	-3.275540	0.136889
F	29.323749	-2.920472	-0.657784
F	31.582527	-1.591501	-0.798102
F	29.145901	2.481795	-1.144066
F	26.891244	1.158183	-1.011280
C	35.278161	1.000623	-1.052105
C	0.622217	1.837158	1.082347
O	-0.425413	0.936250	1.103655
C	-1.591248	1.628333	1.142508
C	-1.325143	2.978819	1.148418
C	0.085549	3.111447	1.107985
C	-2.814476	0.846981	1.169058
C	-2.833488	-0.555416	1.249179
C	-4.029239	-1.262106	1.271470
C	-5.281832	-0.633797	1.221748
C	-5.263015	0.769022	1.150861
C	-4.067144	1.475531	1.123238
F	-1.700041	-1.267274	1.308699
F	-3.957957	-2.601547	1.347086
C	-6.504321	-1.416042	1.252519

O	-7.669520	-0.738307	1.100073
C	-8.714403	-1.641279	1.153573
C	-8.176984	-2.901134	1.343242
C	-6.768527	-2.757887	1.408398
F	-6.397353	1.480773	1.109053
F	-4.137858	2.815329	1.053450
C	-10.015273	-0.968023	1.073951
C	-11.301928	-1.523645	0.909077
C	-12.447785	-0.668868	0.874444
C	-12.348783	0.738739	1.008650
C	-11.041382	1.267981	1.154449
C	-9.939012	0.452230	1.182615
C	-13.751873	-1.194948	0.693253
C	-13.984970	-2.646326	0.514250
N	-12.838318	-3.439259	0.538514
C	-11.529403	-2.980307	0.736559
C	-14.854867	-0.380123	0.672713
C	-14.783736	1.035797	0.831253
C	-13.496547	1.591833	0.991644
C	-13.264914	3.052457	1.118079
N	-11.949456	3.518193	1.242632
C	-10.803822	2.724161	1.280593
C	-16.090345	1.702883	0.804493
O	-17.098337	0.830478	0.440357
C	-18.283378	1.487135	0.503198
C	-18.069611	2.785610	0.906855
C	-16.671750	2.923247	1.096659
O	-9.684806	3.209833	1.407628
C	-11.791607	4.966357	1.356410
O	-14.162422	3.892081	1.113762
O	-10.632902	-3.820871	0.748957
C	-12.991161	-4.882160	0.366041
O	-15.101106	-3.128639	0.353285
C	-19.470784	0.728851	0.153165
C	-19.448761	-0.640861	-0.158183
C	-20.611556	-1.326710	-0.485895
C	-21.870139	-0.709647	-0.523493
C	-21.893248	0.658185	-0.204478
C	-20.729818	1.345287	0.118338
F	-18.306406	-1.340754	-0.150273
F	-20.501633	-2.634742	-0.772033
C	-23.058420	-1.470071	-0.865995
O	-24.221377	-0.778495	-0.961020
C	-25.232916	-1.660106	-1.292138
C	-24.676254	-2.921131	-1.403329
C	-23.290844	-2.800879	-1.129625
F	-23.038261	1.353891	-0.196877
F	-20.840365	2.652176	0.409597
C	-26.538559	-0.992133	-1.340223
C	-27.775935	-1.488220	-1.803096
C	-28.941327	-0.657605	-1.746518

C	-28.890287	0.659964	-1.228429
C	-27.635907	1.137614	-0.777015
C	-26.518670	0.346485	-0.835953
C	-30.201746	-1.112534	-2.209723
C	-30.365411	-2.463333	-2.788183
N	-29.203565	-3.233531	-2.841447
C	-27.936864	-2.844783	-2.382112
C	-31.319399	-0.305733	-2.144332
C	-31.283223	1.005832	-1.622279
C	-30.049057	1.479966	-1.166190
C	-29.924791	2.851553	-0.610169
N	-28.659270	3.271876	-0.178094
C	-27.489640	2.506883	-0.221633
O	-31.441588	-2.887118	-3.198659
C	-29.292323	-4.578581	-3.405562
O	-27.023339	-3.659582	-2.493202
C	-32.554799	1.803019	-1.592639
O	-30.870755	3.630619	-0.512023
C	-28.582137	4.627946	0.359607
O	-26.417221	2.947858	0.176923
H	17.446471	-1.040474	-0.306304
H	20.633168	-5.658992	-0.425359
H	20.776144	-5.272204	1.304758
H	19.151868	-5.203857	0.508895
H	22.635975	4.801895	-1.782793
H	21.039019	4.889388	-2.629180
H	21.121752	5.219747	-0.883432
H	24.334625	0.612201	-1.094074
H	24.526885	-4.125231	-0.563379
H	27.243832	-3.877731	-0.693111
H	31.192383	3.419607	-1.254614
H	33.927093	3.713868	-1.298856
H	0.852981	-0.714431	1.505177
H	4.081922	-5.310813	1.268364
H	4.151666	-4.996552	3.017661
H	2.560237	-4.906653	2.161318
H	6.023284	5.129675	-0.030286
H	4.396622	5.202519	-0.820886
H	4.544132	5.573619	0.912411
H	7.739870	0.963100	0.758290
H	7.992223	-3.588414	2.149969
H	10.695124	-3.388045	1.812912
H	14.497181	3.312757	-1.372099
H	17.200133	3.507664	-1.714254
H	35.996815	1.827792	-1.131825
H	35.471383	0.461221	-0.110958
H	35.462287	0.298643	-1.881205
H	-15.821359	-0.865178	0.526103
H	-12.409060	-5.216472	-0.503956
H	-12.609213	-5.406565	1.253169
H	-14.060239	-5.075456	0.224341

H	-10.718068	5.164381	1.449571
H	-12.209189	5.457333	0.466382
H	-12.339004	5.333134	2.235962
H	-8.968867	0.939519	1.294267
H	-8.745449	-3.817515	1.420806
H	-6.031345	-3.541498	1.550315
H	-2.062206	3.774834	1.176696
H	0.656148	4.029709	1.094959
H	-32.258265	-0.722642	-2.520564
H	-28.608917	-4.669061	-4.261301
H	-28.993293	-5.320058	-2.651459
H	-30.333112	-4.728091	-3.713409
H	-27.539558	4.800866	0.648719
H	-28.905343	5.349801	-0.403520
H	-29.253316	4.724045	1.224581
H	-25.583589	0.778717	-0.475840
H	-25.217071	-3.822016	-1.657892
H	-22.547685	-3.591652	-1.126595
H	-18.832463	3.544794	1.045984
H	-16.138249	3.810631	1.407852
H	-32.451008	2.740626	-2.158385
H	-33.381041	1.208820	-2.009286
H	-32.804694	2.116885	-0.568425

Optimized molecular structures at the B3LYP/6-31G level (atom number and Cartesian coordinates) for tetramer of ThNDIThF$_4$.**

C	-32.207592	1.312483	-0.526806
C	-31.773738	-0.101601	-0.383858
C	-32.703873	-1.165924	-0.461167
C	-34.087507	-0.913546	-0.678293
C	-34.541509	0.497158	-0.820814
N	-33.574206	1.511311	-0.740601
C	-30.440740	-0.355476	-0.150371
C	-29.923878	-1.668138	0.021362
C	-30.821520	-2.749054	-0.095786
C	-32.206748	-2.493109	-0.321887
C	-33.145174	-3.550898	-0.418449
C	-32.719339	-4.967634	-0.311111
N	-31.347479	-5.177007	-0.161706
C	-30.366468	-4.173518	-0.076305
C	-34.484621	-3.286934	-0.624033
C	-34.997908	-1.976893	-0.757442
C	-28.489127	-1.759095	0.344969
S	-27.348451	-0.758773	-0.524239
C	-26.009510	-1.293053	0.477261
C	-26.470070	-2.182291	1.436851
C	-27.853429	-2.440911	1.358292
C	-24.636990	-0.854598	0.242461
C	-23.525501	-1.452031	0.867785

C	-22.222868	-1.033162	0.645463
C	-21.880549	0.022495	-0.220431
C	-22.993281	0.618797	-0.846565
C	-24.296213	0.200637	-0.623535
C	-20.505997	0.453904	-0.458330
S	-19.142918	-0.249408	0.396223
C	-18.002253	0.806533	-0.406121
C	-18.658804	1.638959	-1.285549
C	-20.053772	1.441796	-1.321801
C	-16.560673	0.604248	-0.180023
C	-16.119403	-0.745969	-0.188908
C	-14.797377	-1.106309	-0.059374
C	-13.792034	-0.121443	0.105091
C	-14.213389	1.240364	0.139122
C	-15.585757	1.606469	0.006813
C	-13.207423	2.224371	0.307197
C	-11.886027	1.863126	0.445545
C	-11.447209	0.512811	0.437794
C	-12.420398	-0.487729	0.238254
C	-14.462725	-2.550676	-0.129503
N	-13.103686	-2.858223	-0.070289
C	-12.058604	-1.930141	0.077340
C	-15.944709	3.050841	0.152287
N	-14.899610	3.977075	0.311600
C	-13.541229	3.668622	0.378080
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H	-36.961231	-2.800414	-0.997829

[1] A. D. Laurent, D. Jacquemin, *International J. Quantum Chem.*, **2013**, *113*, 2019-2039.
[2] T. Stein, L. Kronik, R. Baer, *J. Am. Chem. Soc*., **2009**, *131*, 2818.
[3] H. Li, P. Winget, C. Risko, J. S. Sears, J. L. Brédas, *Phys. Chem. Chem. Phys.*, **2013**,*15*, 6293.
[4] L. Pandey, C. Doiron, J. Sears, J. L. Bredas, *Phys. Chem. Chem. Phys.*, **2012**, *14*, 14243-14248.
[5] E. Giussani, D. Fazzi, L. Brambilla, M. Caironi, C. Castiglioni, *Macromolecules*, **2013**, *46*, 2658-2670.
[6] V. Lemaur, L. Muccioli, C. Zannoni, D. Beljonne, R. Lazzaroni, J. Cornil, Y. Olivier, *Macromolecules*, **2013**, *46*, 8171-8178.
[7] J.-L. Brédas, D. Beljonne, V. Coropceanu, J. Cornil, *Chem. Rev.*, **2004**, *104*, 4971.
[8] D. Fazzi, M. Caironi, C. Castiglioni, *J. Am. Chem. Soc.* **2011**, *133*, 19056.
[9] Gaussian 09, Revision **D.01**, 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, J. A. Montgomery, Jr., 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.
[10] N. M. Kirby, S. T. Mudie, A. M. Hawley, D. J. Cookson, H. D. T. Mertens, N. Cowieson, V. Samardzic-Boban, *J. Appl. Cryst*. **2013**, *46*, 1670.
[11] B. C. C. Cowie, A. Tadich, L. Thomsen, *AIP Conf. Proc.* **2010**, *1234*, 307.
[12] B. Watts, L. Thomsen, P. C. Dastoor, *J. Elec. Spec. & Rel. Phen*. **2006**, *151*, 105.
[13] B. Watts, L. Thomsen, P. C. Dastoor, *J. Electron. Spectrosc. Relat. Phenom*. **2005**, *151*, 208.
[14] V. Senkovskyy, R. Tkachov, H. Komber, M. Sommer, M. Heuken, B. Voit, W. T. S. Huck, V. Kataev, A. Petr, and A. Kiriy, *J. Am. Chem. Soc.*, **2011**, *133*, 19966.