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SUPPORTING INFORMATION

Charge Transport in Highly Ordered Organic Nanofibrils: Lessons from Modelling

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Table S1. Experimentally measured and computed drift hole mobilities (in $cm^2V^{-1}s^{-1}$) for several different single-molecule semiconductor assemblies of S- and Se-containing π-conjugated cores. See Scheme S1 for the molecular structures, corresponding to the acronyms and Chart S1 for the types and notations of crystal packing.

Core	Packing type	Experiment		Theory	
		Conditions [a]	μ_+	Method [b]	μ_+
QTH (R=H)	D	Bare SiO_2/Si rt | SC[1]	0.002	MD+kMC[4]	0.022
		HDMS/SiO_2/Si rt | FET[2]	0.011	Dimer DFT[5]	0.021
		OTS/SiO_2/Si rt | FET[3]	0.23		
QTH ($R=C_8H_{17}$)	A	Bare SiO_2/Si rt | FET[6]	0.14		
QTH (R=peptide)	A	Bare SiO_2/Si rt | FET[7]	0.03		
Bp-BTT	D	OTS/SiO_2/Si rt | TFT[8]	0.19	Dimer DFT[9]	0.007
BBTT	C	OTS/SiO_2/Si rt | TFT[8]	0.022	Dimer DFT[9]	0.28
	C	OTS/SiO_2/Ag 30°C[10]	0.008		
BDT	C	Bare SiO_2/Si rt | TFT[11]	0.02-0.05	Dimer DFT[12]	0.23
FPP-DTT	B	OTS/SiO_2/Si rt | TFT[13]	0.15		

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FPP-BDTT	B	OTS/SiO_2/Si rt | TFT[13]	0.0020		
DP-DTT	D	OTS/SiO_2/Si rt | TFT[13]	0.20		
DP-BDTT	D	OTS/SiO_2/Si rt | TFT[13]	0.0026		
Sickle **BBTT**	A	OTS/SiO_2/Si rt | FET[14]	0.20-0.60	MD+kMC[15]	0.55
DBTDT	C	OTS/SiO_2/Si rt | FET[16]	4.7-6.9	MD+kMC[15]	5.61
(R=C_6H_{13})	C	OTS/SiO_2/Si rt | FET[17]	8.5		
	B	OTS/SiO_2/Si rt | FET[17]	18.9		
DBTBT	D	OTS/SiO_2/Si rt | FET[18]	1.8	MD+kMC[4]	0.1
(R=H)					
DITT	B	HMDS/SiO_2/Si | FET [19]	0.0001	MD+kMC[4]	0.0023
BTBT	D	Bare SiO_2/Si rt | FET[20]	0.44-1.71	Dimer DFT[21]	0.031-0.11
(R=$C_{12}H_{25}$)					
BSBS	C	HMDS/SiO_2/Si rt	0.23	Dimer DFT[21]	0.011-0.66
(R=$C_{12}H_{25}$)		| FET[22]		(R=H)	
BTBT (R=Ph)	D	Bare SiO_2/Si rt | FET[23]	0.19-0.22		
		OTS/SiO_2/Si rt | FET[23]	0.36-0.46		
BSBS (R=Ph)	D	Bare SiO_2/Si rt | FET[24]	0.19-0.20		
DNTT	D	OTS/SiO_2/Si rt | FET[25]	1.6-1.8	MD+kMC[4]	0.91

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	D	Cytop/SiO_2/Si rt | FET[26]	8.3	Static DFT[21]	~2.37
				Static DFT/MD[27]	1.8
DNSS	D	OTS/SiO_2/Si rt | FET[25]	0.99-1.9		
PTA	C	Bare SiO_2/Si rt | FET[28]	0.0043	MD+kMC[4]	0.032
				Static DFT[29]	0.89
				with QNT	3.15
HexaTA	C	Bare SiO_2/Si rt | FET[30]	0.0022		

[a] OTS – octadecyltrichlorosilane, HMDS – hexamethyldisilazane, rt – room temperature, SC – single crystal. [b] 'Dimer DFT' methods refers to mobilities, computed on model molecular dimers or clusters using density functional theory (DFT); 'MD' refers to the use of classical molecular dynamics simulations for the optimisation of molecular assembly; 'kMC stands for the computations of transport properties using kinetic Monte Carlo simulations; 'QNT' refers to the inclusion of the full quantum nuclear tunnelling effects in the transfer rate. Detailed discussion of the different methods is given in the manuscript.

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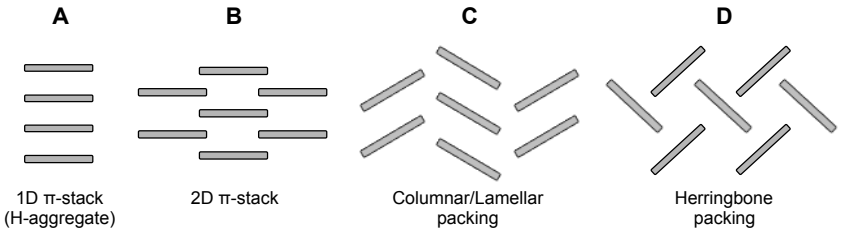
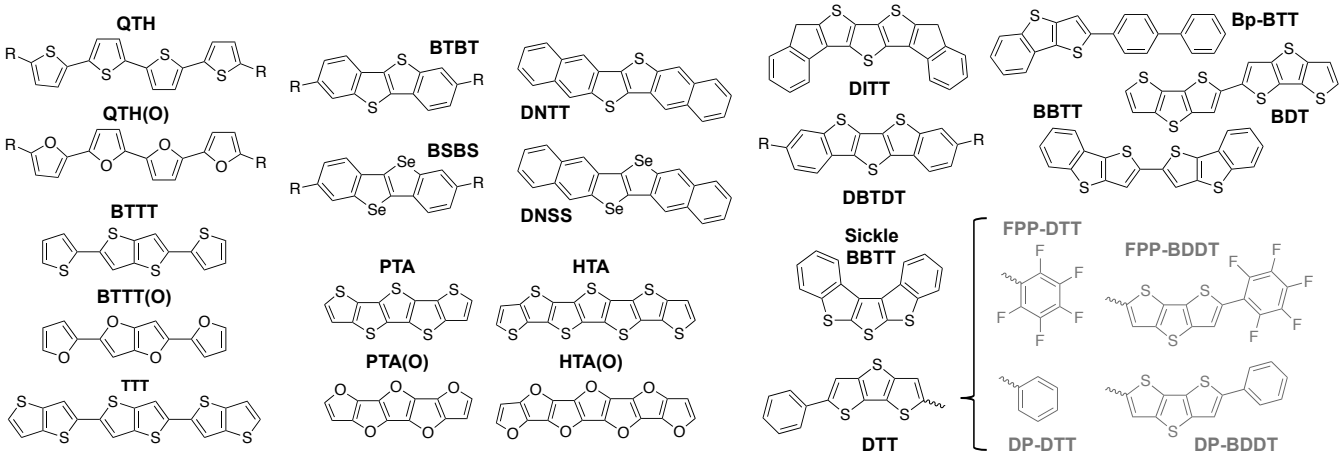


Chart S1. Types of crystal packing.



Scheme S1. Various π-conjugated cores, containing O, S or Se heteroatoms, relevant to organic electronics applications.

Abbreviations:
QTH – 2,2':5',2":5",2"'-quaterthiophene;
QTH(O) – 2,2':5',2":5",2"'-quaterfuran;
BTTT – 2,5-di(thiophen-2-yl)thieno[3,2-*b*]thiophene;
BTTT(O) – 2,5-di(furan-2-yl)furo[3,2-*b*]furan;
TTT – 2,2':5',2"-terthieno[3,2-*b*]thiophene;
BTBT – [1]benzothieno[3,2-*b*][1]benzothiophene;
BSBS – [1]benzoselenopheno[3,2-*b*][1]benzoselenophene;
DNTT – [2,3-*b*:2',3'-*f*]thieno[3,2-b]thiophene; DSTT – [2,3-*b*:2',3'-*f*]selenopheno[3,2-*b*]selenophene;
PTA – thieno[2',3':4,5]thieno[3,2-*b*]thieno[2',3':4,5]thieno[2,3-*d*]thiophene;
PTA(O) – furo[2',3':4,5]furo[3,2-b]furo[2',3':4,5]furo[2,3-d]furan;
HTA – thieno[2",3":4',5']thieno[2',3':4,5]thieno[3,2-b]thieno[2",3":4',5']thieno[2',3':4,5]thieno[2,3-d]thiophene;
HTA(O) – furo[2",3":4',5']furo[2',3':4,5]furo[3,2-*b*]furo[2",3":4',5']furo[2',3':4,5]furo[2,3-*d*]furan;
Sickle BBTT – bis(benzo[4,5]-thieno)[2,3-*b*:3',2'-*d*]thiophene;
DBTBT – dibenzo[d,d']thieno[3,2-b;4,5-b']dithiophene;
Bp_BTT – 2-([1,1'-biphenyl]-4-yl)benzo[*b*]thieno[2,3-*d*]thiophene;
BBTT – α,α'-bis(dithieno[3,2-*b*:2',3'-*d*]thiophene;
DTT – 2-methyl-6-phenyldithieno[3,2-b:2',3'-*d*]thiophene.

Table S2. HOMO energies and HOMO-LUMO gaps (eV) of the investigated cores, computed at the PBE0/def2SVP level of theory.

Core	E_{HOMO}	HLG
QTH	-5.43	3.47
QTH(O)	-4.97	3.67
TTT	-5.48	3.44
PTA	-5.75	4.18
PTA(O)	-5.37	4.39
HTA	-5.58	3.75
HTA(O)	-5.18	3.90

Table S3. Vertical and adiabatic ionisation potentials and electron affinities, as well as the reorganisation energies (all in eV), corresponding to the hole and electron transfer, computed from the PBE0/def2SVP electronic energies.

Core	*IP*		λ_+	*EA*		λ_-
	vertical	adiabatic		vertical	adiabatic	
			E_e			
QTH	6.63	6.44	0.34	-0.78	-0.94	0.29
QTH(O)	6.47	6.34	0.28	-0.14	-0.28	0.29
TTT	6.58	6.39	0.33	-0.95	-1.12	0.30
PTA	7.08	6.92	0.31	-0.25	-0.38	0.27
PTA(O)	6.89	6.74	0.30	0.50	0.30	0.46
HTA	6.73	6.59	0.28	-0.68	-0.79	0.23
HTA(O)	6.51	6.37	0.29	0.01	-0.17	0.39

Table S4. Computed effective transfer integrals (electronic couplings) V (PBE0-dDsC/DZP, in eV), hopping rates k (in s^{-1}), mobilities μ (in $cm^2V^{-1}s^{-1}$), DORI compactness indices (isovalue α=o.96, PBE0-dDsC/DZP densities), interplanar distances d, longitudal and transversal shifts (all in Å) in the PBE0-dDsC/def2SVP optimised cofacial and antifacial dimer geometries.

Core	V_+	V_-	k_+	k_-	μ_+	μ_-	DORI index [a]	d	shift	
									long.	trans.
					cofacial					
QTH	0.11	0.12	1.4×10^{13}	2.4×10^{13}	0.307	0.510	0.75	3.31	1.41	0.84
QTH(O)	0.02	0.09	9.1×10^{11}	1.7×10^{13}	0.019	0.344	0.54	3.26	1.36	0.55
TTT	0.19	0.04	4.3×10^{13}	3.0×10^{12}	0.922	0.064	0.93	3.33	1.44	0.66
PTA	0.29	0.00	1.3×10^{14}	2.8×10^{10}	2.653	0.001	0.69	3.28	1.88	0.04
PTA(O)	0.16	0.12	4.6×10^{13}	4.0×10^{12}	0.906	0.079	0.48	3.18	1.58	0.03
HTA	0.33	0.02	2.3×10^{14}	1.1×10^{12}	4.778	0.024	0.97	3.28	1.82	0.02
HTA(O)	0.20	0.10	7.8×10^{13}	6.7×10^{12}	1.524	0.131	0.67	3.17	1.27	0.02
					antifacial					
QTH	0.22	0.09	5.4×10^{13}	1.3×10^{13}	1.181	0.285	n/a	3.37	0.20	1.39
QTH(O)	0.03	0.33	1.7×10^{12}	2.1×10^{14}	0.033	3.978	0.61	3.16	0.07	1.03
TTT	0.05	0.11	2.5×10^{12}	1.9×10^{13}	0.053	0.420	n/a	3.34	1.13	0.24
PTA	0.37	0.03	2.2×10^{14}	1.7×10^{12}	4.679	0.037	0.69	3.33	0.29	0.04
PTA(O)	0.17	0.11	5.2×10^{13}	3.7×10^{12}	1.031	0.075	0.48	3.21	0.75	0.22
HTA	0.40	0.04	3.4×10^{14}	7.1×10^{12}	7.173	0.152	0.98	3.31	0.14	0.05
HTA(O)	0.22	0.12	8.9×10^{13}	8.2×10^{12}	1.762	0.163	0.66	3.19	0.62	0.09

[a] In several species, the intermolecular DORI domains with 0.95 isovalue are merged with the intramolecular S–S domains, hence the compactness indices for these domains cannot be compared to the rest of the systems and therefore are not reported.

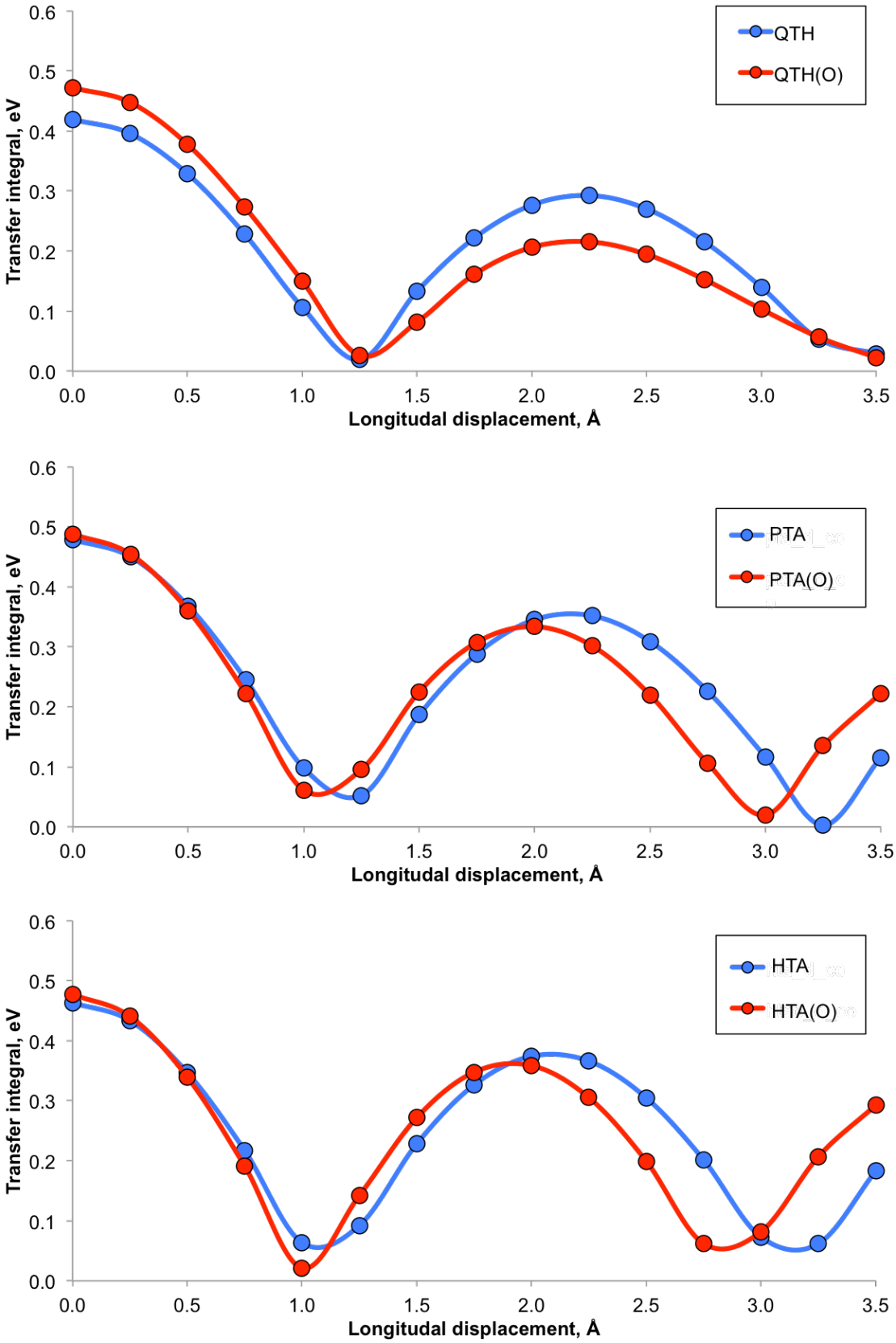


Figure S1. Computed hole transfer integrals (PBE0-dDsC/DZP) for the cofacial dimers of QTH (d = 3.38Å, l_{trans} = 0.0) and QTH(O) (d = 3.26Å, l_{trans} = 0.0), PTA (d = 3.28Å, l_{trans} = 0.0) and PTA(O) (d = 3.18Å, l_{trans} = 0.0), HTA (d = 3.28Å, l_{trans} = 0.0) and HTA(O) (d = 3.17Å, l_{trans} = 0.0) at a range of longitudinal shifts.

Including peptide side chains in the reorganisation energies and electronic couplings

The reorganisation energies, computed according to Eq. 4 of the manuscript using the PBE0/def2-SVP method for PTA cores with different substituents, are:

- with H atoms instead of the side chains λ_+=0.31 eV;
- with CH_3 groups instead of the side chains λ_+=0.30 eV;
- with monopeptide side chains, in which the chains beyond their first methylene group (directly bound to the PTA core) were frozen to mimic the constrain within the lateral H-bonding network of the fibril, λ_+=0.30 eV;
- with monopeptide side chains (fully optimised) λ_+=0.39 eV. This value is higher due to geometrical changes (Figure S2A).

It is thus evident that the bare core yields the lower limit estimate of the reorganisation energy, *i.e.* the upper limit of the charge mobility. This estimate is likely to be realistic provided the species are reasonably constrained within the nanofibril. A more accurate determination of the reorganisation energy within the nanofibril (e.g. tetramer, as opposed to the isolated monomer) is challenging in terms of unambiguous choice of the system size and technical implementation.

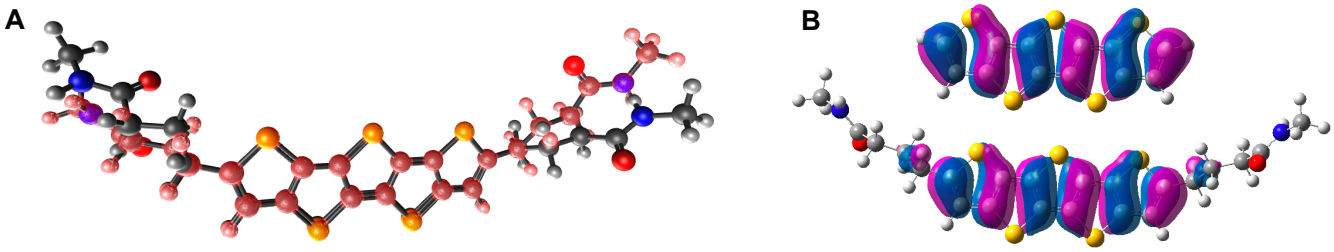


Figure S2. (A) PBE0/def2-SVP optimised geometries of the neutral and cation radical PTA cores with monopeptide side chains. (B) PBE0/def2-SVP HOMO plots of fully relaxed neutral PTA cores with R=H (top) and R=monopeptide (bottom).

Geometry of the PTA dimer bearing monopeptide side chains (in their extended conformations) was optimised using the PBE0-dDsC/def2SVP method. This optimised geometry was then used to generate the geometries of two analogues with –H and –CH_3 groups instead of the H-bonding side chains, which were not re-optimised so as to keep the relative alignment of the cores identical in all three systems. The hole transfer integrals for these three dimers were computed at the PBE0-dDsC/DZP level as implemented in ADF[31] and compared to that of a fully relaxed PTA dimer (R=H). These

[31] **ADF2014**, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com. E. J. Baerends, T. Ziegler, J. Autschbach, D. Bashford, A. Bérces, F. M. Bickelhaupt, C. Bo, P. M. Boerrigter, L. Cavallo, D. P. Chong, L. Deng, R. M. Dickson, D. E. Ellis, M. van Faassen, L. Fan, T. H. Fischer, C. Fonseca Guerra, M. Franchini, A.

computations rely upon monomer orbitals treated as charge localised states and thus lack polarisation by the partner monomer and environment. To validate the applicability of this assumption to selected system (PTA), we have employed the Frozen Density Embedding (FDE) scheme[32] at the PW91/TZP level, as implemented in ADF.[31]

Table S5. Computed charge transport and geometry parameters of the PTA cores with different side chains (using λ_+=0.31 eV).

Core [a]	Level of theory	V_+, eV	k_+, s^{-1}	μ_+, $cm^2V^{-1}s^{-1}$	d, Å	shift, Å	
						long.	trans.
opt. R=H	PBE0/DZP	0.29	1.3×10^{14}	2.65	3.28	1.88	0.04
fde R=H	PW91/TZP	0.27	1.1×10^{14}	2.29	3.28	1.88	0.04
fr. R=H	PBE0/DZP	0.27	1.2×10^{14}	2.54	3.34	2.66	0.18
fr. R=CH_3	PBE0/DZP	0.28	1.2×10^{14}	2.58	3.34	2.66	0.18
opt. R=pept	PBE0/DZP	0.28	1.3×10^{14}	2.70	3.34	2.66	0.18
opt. R=pept	PBE0/TZP	0.28	1.2×10^{14}	2.62	3.34	2.66	0.18
opt. R=pept	PW91/DZP	0.25	9.4×10^{13}	2.03	3.34	2.66	0.18
opt. R=pept	PW91/TZP	0.24	9.2×10^{13}	1.99	3.34	2.66	0.18
fde R=pept	PW91/TZP	0.21	6.8×10^{13}	1.47	3.34	2.66	0.18

[a] 'opt.' stands for fully optimised dimer, 'fde' stands for FDE scheme used to compute the electronic couplings for the dimer in its fully optimised geometry, 'fr.' refers to the frozen alignment of the cores, taken from the optimised geometry of the dimer with the monopeptide side chains.

The transfer integrals are relatively similar for all investigated dimer systems, despite fairly different longitudinal shifts in the dimers with no and with H-bonding side chains. This feature is likely to be system-dependent (see Figure S1). The similarity between the transfer integrals of the bare and peptide-flanked core dimers is in agreement with the fact that the corresponding monomer orbitals are nearly identical (Figure S2B). The difference between the results, obtained using localised monomer orbitals and the FDE numbers can potentially be attributed to the influence of the level of theory (PBE0 *vs.* PW91).

Ghysels, A. Giammona, S. J. A. van Gisbergen, A. W. Götz, J. A. Groeneveld, O. V. Gritsenko, M. Grüning, S. Gusarov, F. E. Harris, P. van den Hoek, C. R. Jacob, H. Jacobsen, L. Jensen, J. W. Kaminski, G. van Kessel, F. Kootstra, A. Kovalenko, M. V. Krykunov, E. van Lenthe, D. A. McCormack, A. Michalak, M. Mitoraj, S. M. Morton, J. Neugebauer, V. P. Nicu, L. Noodleman, V. P. Osinga, S. Patchkovskii, M. Pavanello, P. H. T. Philipsen, D. Post, C. C. Pye, W. Ravenek, J. I. Rodríguez, P. Ros, P. R. T. Schipper, G. Schreckenbach, J. S. Seldenthuis, M. Seth, J. G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T. A. Wesolowski, E. M. van Wezenbeek, G. Wiesenekker, S. K. Wolff, T. K. Woo, A. L. Yakovlev.

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Energy decomposition analysis

The energy decomposition analysis of selected dimers for a range of longitudinal displacement values (0.0-3.5 Å, step = 0.25 Å) at fixed intermolecular distances (equal to those in the optimised PBE0-dDsC/def2SVP geometries) was performed using the simplest truncation of the symmetry-adapted perturbation theory[33] (SAPT0) with the jun-cc-pVDZ basis set employing the density fitting algorithm (DF-SAPT),[34] implemented in the Psi4-Beta5 code.[35] For the distributed multipole analyses (DMA),[36] the atom-centered multipoles up to the 8th order were generated using Molpro[37] at the HF/6-311G** level. The interaction energies between these multipoles were computed up to the 5th order using an in-house program of the Sherrill research group (Georgia Institute of Technology). The difference between the SAPT0 electrostatic energy and the DMA interaction energy was used to elucidate the effect of 'charge penetration'.[38]

As seen in Figure S3 below, there is a pronounced minimum of the longitudinal shift of the HTA dimer around 1.5-2.5 Å, at which the interaction energy is at its lowest due to minimised exchange and electrostatic components. In turn, the extremum in electrostatic energy with the lateral shift arises primarily from the charge penetration effect, indicative of maximised orbital rather than through-space Coulombic interaction at this shift. In contrast, the interaction energy profile of the oxygen analogue, HTA(O), is much flatter (1-3 Å), and the charge penetration is gradually decreasing with the decreasing spatial overlap between the cores (increasing shift). The absence of an extremum in this profile indicates attenuated orbital interaction compared to HTA.

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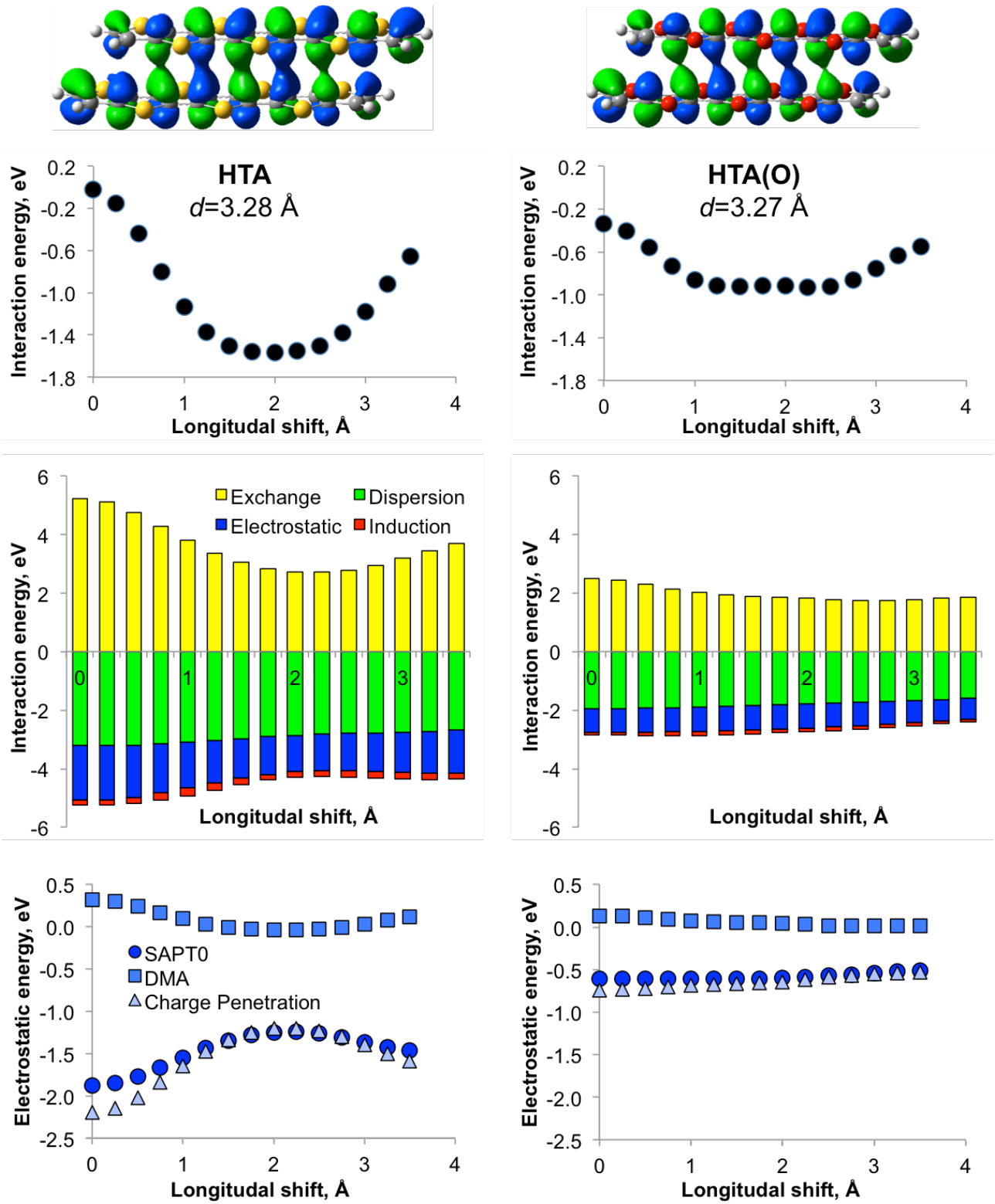

Figure S3. Results of energy decomposition analysis of HTA and HTA(O) dimers with monomers, shifted along the long axis. Plots of HOMO-1 with 0.02 isovalue are shown.

Table S6. Computed electronic energies (at the PBE0-D3BJ/def2SVP level, all in Hartrees) for the neutral, cation radical and anion radical cores in the optimised and 'frozen' geometries.

geometry	0,1	0,1	+1,2	+1,2	0,1	–1,2	–1,2
charge, multipl.	0,1	+1,2	+1,2	0,1	–1,2	–1,2	0,1
Core				E_e			
QTH	-2206.32702	-2206.08354	-2206.09028	-2206.32142	-2206.35563	-2206.36166	-2206.32224
QTH(O)	-914.90779	-914.66990	-914.67495	-914.90264	-914.91297	-914.91826	-914.90250
BTTT	-2129.05265	-2128.80208	-2128.80935	-2129.04700	-2129.07418	-2129.08076	-2129.04770
BTTT(O)	-837.61112	-837.36889	-837.37408	-837.60595	-837.61251	-837.61826	-837.60541
TTT	-3077.08355	-3076.84168	-3076.84855	-3077.07820	-3077.11837	-3077.12465	-3077.07885
PTA	-2448.52019	-2448.26012	-2448.26579	-2448.51463	-2448.52925	-2448.53414	-2448.51529
PTA(O)	-834.15392	-833.90060	-833.90609	-834.14848	-834.13573	-834.14295	-834.14432
HTA	-3396.55125	-3396.30384	-3396.30903	-3396.54613	-3396.57612	-3396.58042	-3396.54693
HTA(O)	-1136.43013	-1136.19080	-1136.19613	-1136.42486	-1136.42975	-1136.43655	-1136.42269

Modelling of the nanofibrils and MD simulations

Constructing the nanofibrils. The strategy used to generate helical shape nanofibrils is summarised in Figure S4, and the details are given below.

Monomers: π-stacked cores flanked with oligopeptides comprised of four alanine (ALA) residues were built manually using a combination of Avogadro[39] and VMD[40], constraining ALA residues onto a beta-sheet configuration in the Ramachandran dihedral space to form the H-bond aggregators. Then, monomer structures were roughly optimised with the UFF force-field[41] before being used as an input into AmberTools14[42] and the antechamber command.

Dodecamers: From a monomer, dodecameric structures were generated by replicating monomers along the perpendicular axis of the core at a distance of 0.5 nm. Then, an energy minimisation, an NPT equilibration and finally an MD run of 10 ns were performed to relax the dodecameric structure in explicit solvent. Parameters for each run were the same as the ones described in the main text.

Fibrils: In order to generate the nanofibrils, the most representative dimer structure was extracted from the MD run of the corresponding dodecamer structure. Then, dimers were replicated and rotated along the axis formed by the centre of mass of each core of the dodecamer (which also corresponds to the direction of the H-bond aggregators) to reproduce a helical shape. Four MD runs of 10 ns were performed to relax the nanofibrils (made of central cores with S atoms), with initial configurations corresponding to helical structures with a periodicity *P* of 30, 60, 90 and 120 nm (Table S7). This sampling of periodicity leads to unit cells with different box parameters and different numbers of monomers to get one turn (Table S8). The turn was chosen to be a left turn by default. The radius between the center of mass of each core for all the fibrils was chosen to be zero, initially. It means that the long axis of the nanofibril is completely straight and oriented along the z-axis at t = 0. However, as shown in Figure S4 for the case of PTA cores with P = 30 nm, the radius is strongly relaxed during the MD run.

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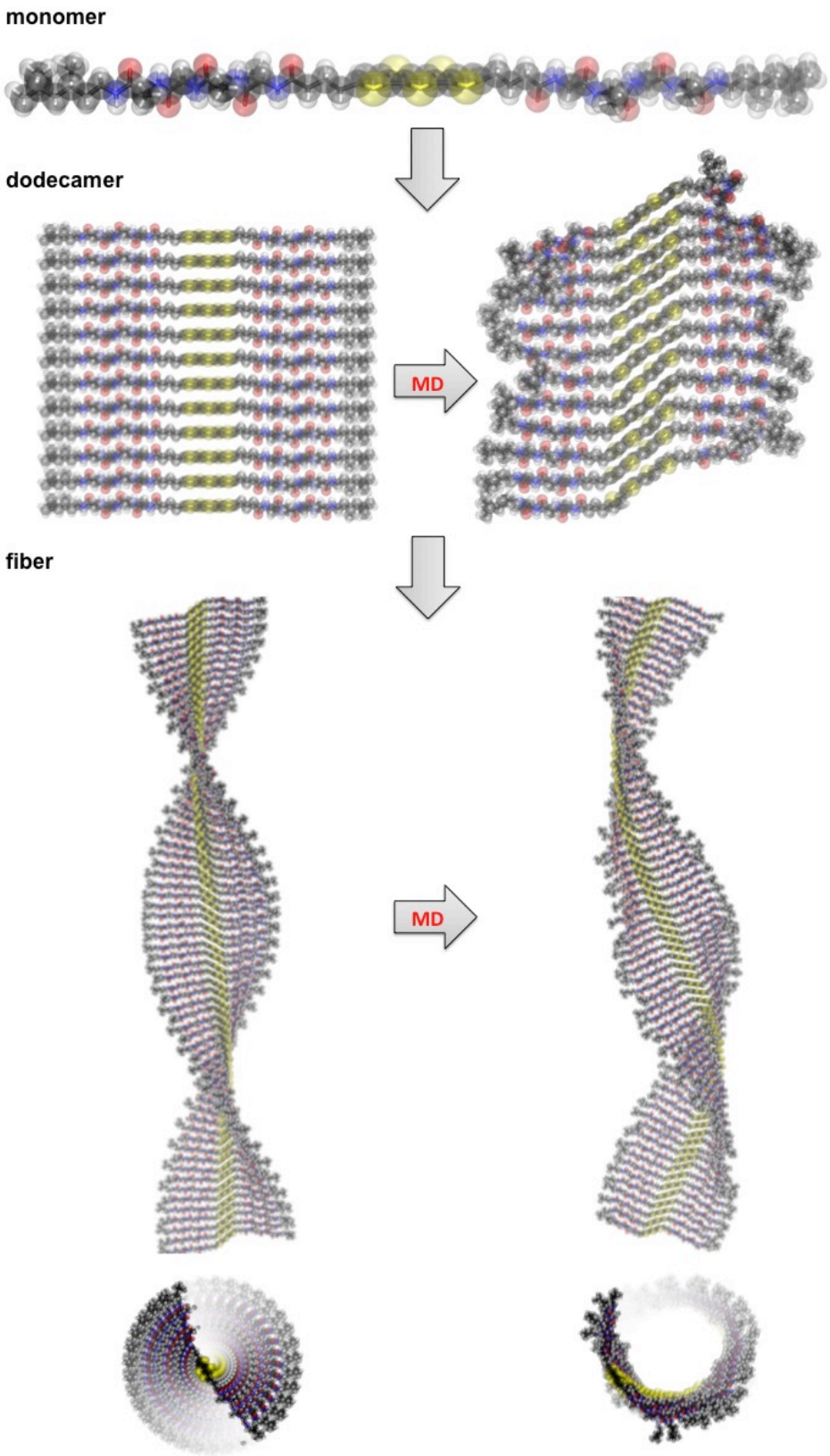

Figure S4. Modelling strategy used in the present work to generate the nanofibrils. Atomic structures at the different stages of the process are shown in VDW representation. For the dodecamer and the nanofibril structures, left panels represent the initial configuration and right panels correspond to structures relaxed after 10 ns MD simulations.

Table S7. MD simulations of the nanofibrils and their corresponding structural stabilities. S and B correspond to stable and broken nanofibrils, respectively. * corresponds to MD runs of the nanofibrils that were selected for CT calculations.

	PTA	HTA	QTH	TTT	PTA(O)	HTA(O)	QTH(O)
P = 30 nm	S*	B	B	B	S*	S*	B
P = 60 nm	S	S*	B	S*	-	S	B
P = 90 nm	B	B	B	S	-	-	B
P = 120 nm	B	B	S*	B	-	-	B
P = 45 nm	-	-	-	-	-	-	B
P = 75 nm	-	-	-	-	-	-	S*
P = 105 nm	-	-	-	-	-	-	B

Table S8. MD simulations parameters of the nanofibrils used for CT calculations. P represents the periodicity of the nanofibril; L_x, L_y and L_z represent the simulation box parameters; N_m represents the number of monomers per turn and the number in parenthesis corresponds to the number of atoms per monomer; N_s represents the number of solvent molecules and N_{tot} represents the total number of atoms in the simulation box.

	P (in nm)	$L_x = L_y$ (in nm)	L_z (in nm)	N_m	N_s	N_{tot}
PTA	30	16.1	29.6	70 (181)	38215	318 390
HTA	60	16.5	59.2	134 (187)	84927	704 474
QTH	120	16.4	118.4	248 (190)	170410	1 410 400
TTT	60	16.7	59.5	132 (192)	88981	737 192
PTA(O)	30	15.6	29.5	66 (181)	38238	317 850
HTA(O)	30	16.0	29.6	68 (187)	39979	332 548
QTH(O)	75	16.3	74.0	156 (190)	104828	868 264

For central cores with O atoms, only two periodicities were tested: the same as the one obtained for the sulfur case, and a smaller one. For example, for the case of HTA(O), the periodicity of 60 nm was tested first, leading to a stable structure. Then, the periodicity of 30 nm was tested and the most stable nanofibril was selected. For the case of QTH(O), it was more complicated due to the fact that periodicities of 30, 60, 90 and 120 nm led to broken fibrils. Therefore, a larger sampling was performed, with intermediate values of P: 45, 75 and 105 nm. Finally, only P = 75 nm led to a stable structure (see Table S7 for a complete summary of the sampling).

Estimation of the relative alignment of π-stacked cores. The interplanar distance d and the longitudinal and transversal shifts between the consecutive cores (shown in Figure 3 of the manuscript)

have been extracted from the MD simulations as explained in the previous work[43]. Values in Table 1 of the manuscript correspond to the most representative configurations, *i.e.* the global minimum of the free-energy profiles and surfaces.

Structural stability of nanofibrils. The global stability of each nanofibril during MD simulations was established using two distinct criteria. First, to estimate if a structure was broken or not during the MD simulations, we computed the distances between N atoms of the first alanine residues of the left and of the right side chain of two consecutive residues, as depicted in Figure S5A. These distances represent the "quality" of the H-bond aggregation between the oligopeptides. As shown in Figure S5B for the case of PTA nanofibrils, structures with periodicities of 90 and 120 nm are broken during the MD runs, with distances between consecutive monomers as large as 20 Å. On the opposite, fibrils with a periodicity of 30 or 60 nm show relatively constant distances as a function of time, around 4-5 Å, reflecting a strong interaction between the aggregators. Therefore, to differentiate between the two former cases, another criterion was required. Root-Mean Square Deviation (RMSD) for all the heavy atoms (all atoms except H atoms) was computed for the nanofibrils to validate the previous criterion (Figure S5C). The nanofibril showing the lowest deformation during its MD run (in the case of PTA cores, P = 30 nm) was selected as the "best case" nanofibril and was then used to compute the CT properties. The MD relaxation of these selected nanofibrils for each core is shown in Figure S6.

Influence of the periodicity on CT mobilities. In order to test the influence of the periodicity on the CT mobilities, MD simulations of the nanofibrils with 2 turns were performed. Two different cores (one with S and one with O atoms, both with a periodicity of 30 nm) were tested, *i.e.* PTA and HTA(O). As shown in Figure S7, adding a second turn to the CT calculations (from 30 to 60 nm length), which increases the number of consecutive monomers by a factor of two, does not change significantly the CT properties. In fact, the widths and heights of the distribution $P(\mu)$ are very similar, showing that the disorder is quantitatively the same. In addition, the average mobilities went from 1.9-2.0 to 2.2, which corresponds to the same order of magnitude.

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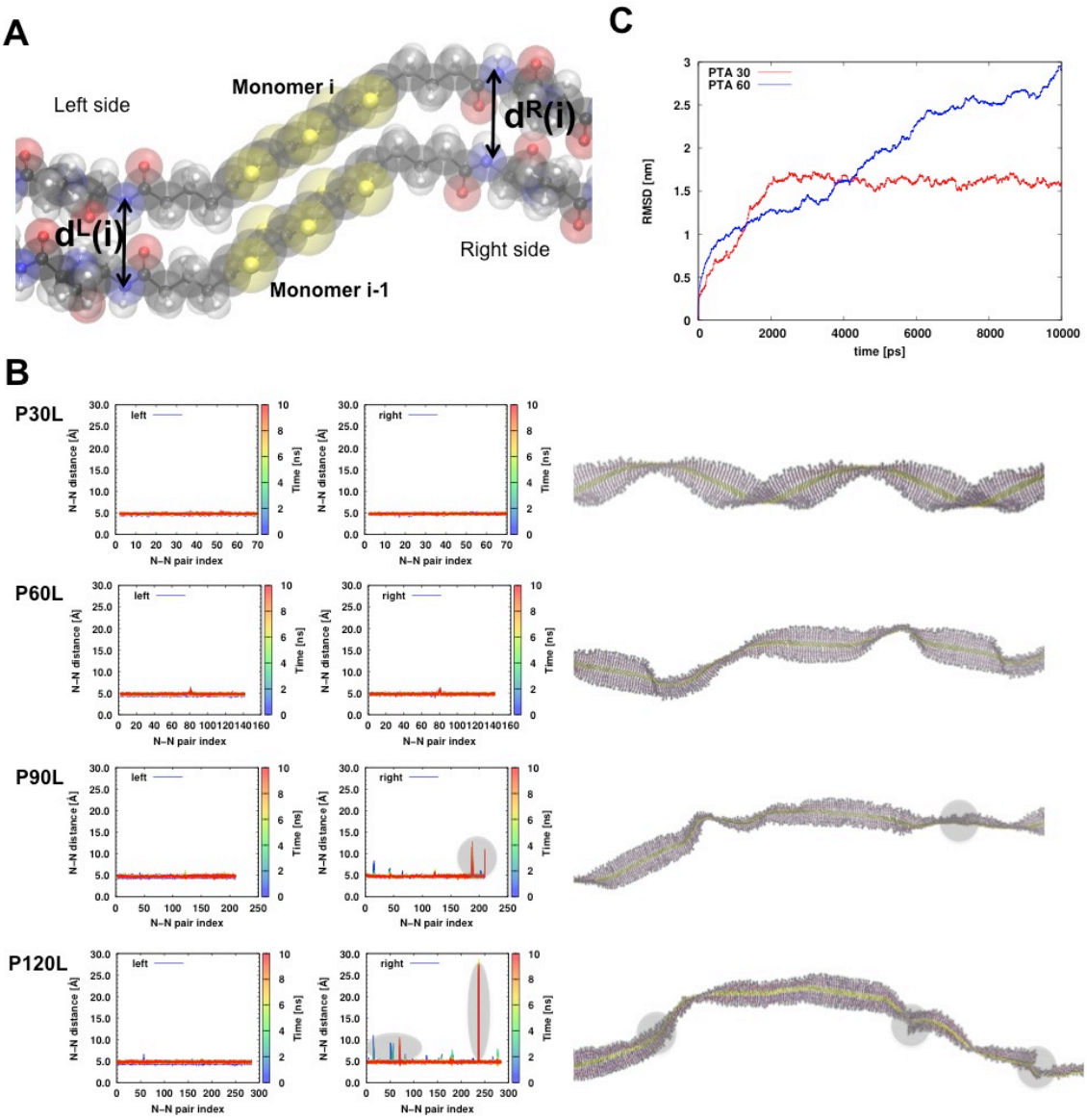

Figure S5. Structural stability of nanofibrils during the MD simulations. (A) Schematic representation of the distance between N atoms of two consecutive monomers used to characterise the stability of the H-bond network between aggregators. (B) Distances as a function of time and dimer positions during MD simulations of the PTA nanofibrils with periodicities P = 30, 60, 90 and 120 nm. Atomic structures of the corresponding nanofibrils at the end of each MD run are shown on the right. Grey areas correspond to broken aggregates. (C) Root-mean square deviation (in nm) of PTA nanofibrils with P = 30 (red) and P = 60 nm (blue) computed for all heavy atoms (all atoms except H atoms) during 10 ns MD simulations.

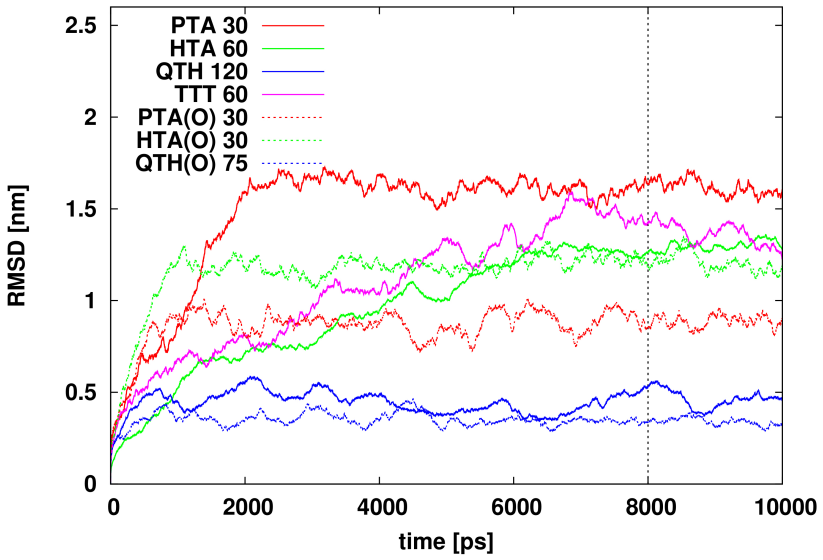

Figure S6. RMSD (in nm) of selected nanofibrils during 10 ns MD simulations. The dashed line indicates the part of the trajectory used for CT calculations (from 8 to 10 ns).

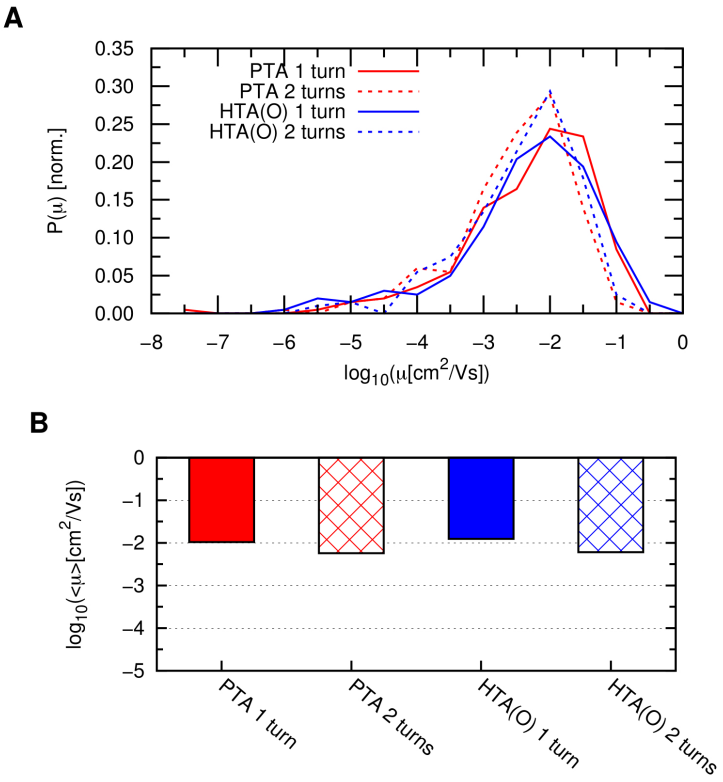

Figure S7. Influence of the periodicity on the CT properties. (A) Probability distribution function of mobilities μ. (B) Averaged mobilities $<\mu>$.

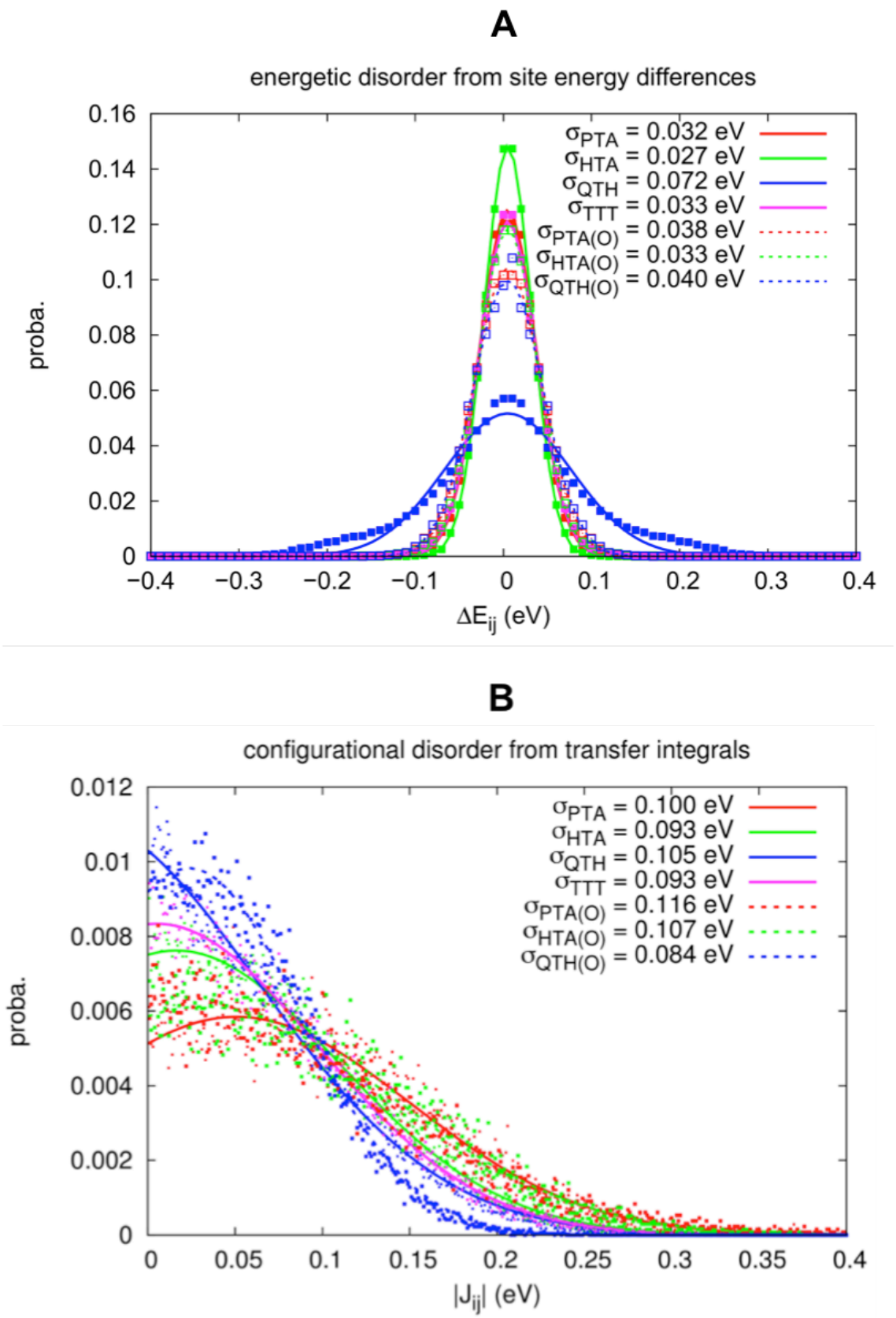

Figure S8. Distributions of site energy differences (energetic disorder, A) and transfer integrals (configurational disorder, B) for the neighbour pairs in the PTA (most stable) and QTH (least stable) fibrils.

Comparison of ZINDO and DFT transfer integrals

The transfer integrals between all the neighbouring sites were computed with a semiempirical ZINDO method and a more time-demanding DFT method (PBE0/def2-SVP) for a single snapshot of the pentathienoacene nanofibril. ZINDO values are evaluated with VOTCA software[44] based on the HOMO orbitals computed using Gaussian 09,[45] while the DFT values were computed with VOTCA coupled to Turbomole 6.5.[46] The comparison of transfer integrals is given in Figure S9.

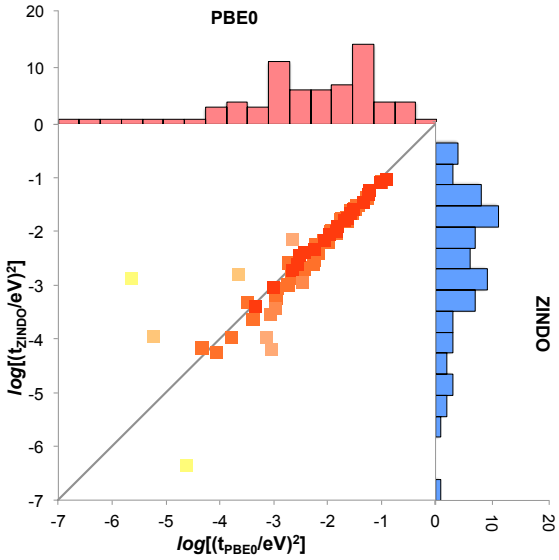

Figure S9. Distribution of transfer integrals computed with ZINDO and PBE0/def2-SVP methods.

There is a good agreement between the ZINDO and PBE0 values with a slight underestimation of the transfer integrals when ZINDO is used. The agreement is somewhat deteriorated for the smaller transfer integrals, which has also been reported in ref 44. Overall, the computed hole mobilities (with all other parameters fixed, as detailed in the Computational Details section of the manuscript) are 8.7×10^{-4} $cm^2V^{-1}s^{-1}$ from ZINDO and one order of magnitude larger, 4.8×10^{-3} cm^2 $V^{-1}s^{-1}$ with PBE0.

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APPENDIX 1

Optimised geometries of all monomers (PBE0/def2-SVP) and dimers (PBE0-dDsC/def2-SVP) in the form of Cartesian coordinates.

QTH

0 1
S 0.3745735907 1.0505417077 5.8211417645
C 0.0357319064 -0.1262152742 4.592272548
C -0.2160220585 -1.3592999409 5.1603217752
C -0.1417042187 -1.3437710224 6.5768991608
C 0.1635855497 -0.103599943 7.074449754
C 0.0468303371 0.2428497667 3.1958367903
C 0.0332223816 1.5022649511 2.6292516581
C 0.0392913686 1.4793857533 1.2173081192
C 0.0569007612 0.2013113109 0.6920109053
S 0.0896295938 -0.9782534601 1.9645963325
C 0.0570704523 -0.2109204021 -0.6891773514
S 0.3457929748 0.9420502294 -1.953778216
C 0.163891186 -0.2604604923 -3.190615159
C -0.0843443496 -1.498204935 -2.6304987869
C -0.1443129357 -1.4708701575 -1.2199083242
C 0.2825530519 0.0995568615 -4.5843932036
C 0.2713597264 1.355198728 -5.1586904181
C 0.4097641244 1.3216289031 -6.5701290988
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H 6.441305 -1.460898 -2.779469
H 7.230688 -1.528643 -0.138234

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C 0.0355731764 -1.2928067189 -4.5464032147
C 0.0175126856 -0.9803180513 -5.9301992024
C -0.0450842397 0.3686721517 -6.1645850729
C -0.0118360464 -0.0990184552 -2.2961922209
C 0.25132971 0.9947923719 -1.496641349
C 0.1610113325 0.6679561099 -0.1232427329
C -0.1653806197 -0.6675756865 0.1232240324
S -0.3826162115 -1.5298682042 -1.3576883597
C -0.2556990051 -0.9944119487 1.4966226489
C 0.0074668138 0.0993988617 2.2961735216
S 0.3782469288 1.5302486258 1.3576696593
C 0.0106986008 0.1741349448 3.7393983867
S 0.0932097335 -1.2662845978 4.7023228406
C 0.040716358 -0.3682917579 6.1645663708
C -0.0218818021 0.9806983929 5.9301805231
C -0.0399429111 1.2931870622 4.5463845427
H -0.5187707755 -1.9739135097 1.8963830258
H 0.5144014283 1.9742939487 -1.8964017223
H -0.0610339585 1.7261240015 6.7251244239
H -0.1068437662 2.3061449735 4.1463647126
H 0.1024735336 -2.3057646527 -4.1463833585
H 0.0566648826 -1.7257436766 -6.7251430856
H 0.0619043307 -0.8862279283 7.1222127276
H -0.0662712476 0.8866083481 -7.1222314368

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C -0.0629607432 -1.3037774554 -4.5201888002
C -0.0298405659 -0.9876093069 -5.8847505992
C 0.0703923648 0.3750706819 -6.1043089558
C 0.0059426097 -0.1211147349 -2.2831215631
C 0.0829800273 1.0277012676 -1.472340158

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C 0.012379443 -0.1807562611 -3.737029489
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C 0.0071600412 -0.1081366224 -2.3230445199
C 0.0825070613 1.0213781152 -1.4893525438

C 0.0493644089 0.6998715349 -0.1265952058
C -0.0537335969 -0.699491147 0.1265765036
S -0.1083073077 -1.5998501778 -1.3465771339
C -0.0873492153 -1.0273208798 1.4723214558
C -0.0103117978 0.1214951227 2.2831028609
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C -0.016748631 0.181136649 3.7370107868
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C -0.0740348599 -0.3665278338 6.1989855646
C 0.0248344333 0.9809438247 5.9478697514
C 0.0579839446 1.302083092 4.5720734255
H -0.1628621447 -2.0335420532 1.8880474148
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H 0.073089201 1.7291223284 6.7425644532
H 0.1339678344 2.3162077095 4.1773057892
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H 0.1142075521 0.8809673006 -7.1571946876

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C -4.273735 -1.580324 0.163589
C -5.107354 -2.061482 -0.824543
C -6.477722 -1.816154 -0.561636
C -6.674581 -1.152340 0.620275
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C -2.004646 -1.048336 1.163681
C -0.648630 -1.341298 0.905989
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S -1.943529 -2.547566 -0.961563
C 0.914855 -2.408806 -0.490152
C 1.744284 -1.816747 0.439726
S 0.851342 -0.928050 1.646982
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H -7.614997 -0.832351 1.065459
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C -4.022116 1.224718 -1.398909
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S 1.942939 2.547572 0.962194

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C -5.358978 -2.071281 0.813114
C -1.550310 -1.806366 0.063083
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C 0.659795 -1.611486 0.694894
C 0.812230 -1.626553 -0.689072
S -0.716122 -1.771962 -1.472561
C 2.151567 -1.519737 -1.120530
C 3.022028 -1.423307 -0.056901
S 2.188554 -1.458722 1.478729
C 4.459385 -1.313100 -0.089939
S 5.311735 -1.216201 -1.594578
C 6.832227 -1.138417 -0.805810
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C 5.344947 -1.284294 0.965894
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C 0. 1.2046878715 -1.2762854938
C 0. 0.0687058197 -2.0669348433
O 0. -1.0820938251 -1.3235795424
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C 0. 0.0932725002 3.4908314613
H 0. 2.2285126981 -1.6377407285
C 0. -0.0932725002 -3.4908314613
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H 0. 1.2845529227 6.558642153
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C 0. 0.0485605556 -2.0556603778
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H 0. 2.2317704147 -1.6213915194
C 0. -0.0941743644 -3.4537042529
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C 5.281292 1.216907 -1.115430
C -3.282940 1.918270 1.231928
C -4.602416 2.089165 0.724374
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H 0.597383 -1.900282 2.160327
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antifacial
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H -4.531490 1.302834 2.299810
H -7.142616 1.186055 1.408314
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C 0.2609726646 -1.0972845301 1.4211749998
C 0.1681206555 -0.6738133955 0.0754751904
C -0.1692615092 0.673713402 -0.0754773161
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H 6.270818 1.874696 1.657346
H -7.752877 1.417984 -0.995472
H 6.977478 1.914506 -0.991634