Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information to: First-principles study of nanothreads derived from five-membered heterocyclic rings: thiophene, furan and pyrrole

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1. Additional results

1.1. Phosphole-derived nanothreads

Figure S1 shows the structure of phosphole-derived nanothreads, along with their electronic band structure and density of states. As stated in the main text, phosphole is not stable at normal conditions,[1] and the structure of its nanothreads may not follow the proposed *syn*, *anti* and *syn-anti* configurations. However, in order to provide a first insight into the feasibility of phosphole-derived materials, as well as to compare their electronic and mechanical properties with those of similar nanothreads, we investigated the structures shown in Figure S1, which are in good agreement with experimental data in the cases of furan[2] and thiophene.[3] We note that the phosphole-derived nanothreads are similar to those of pyrrole, which were presented in the main text, but with P atoms instead of N.

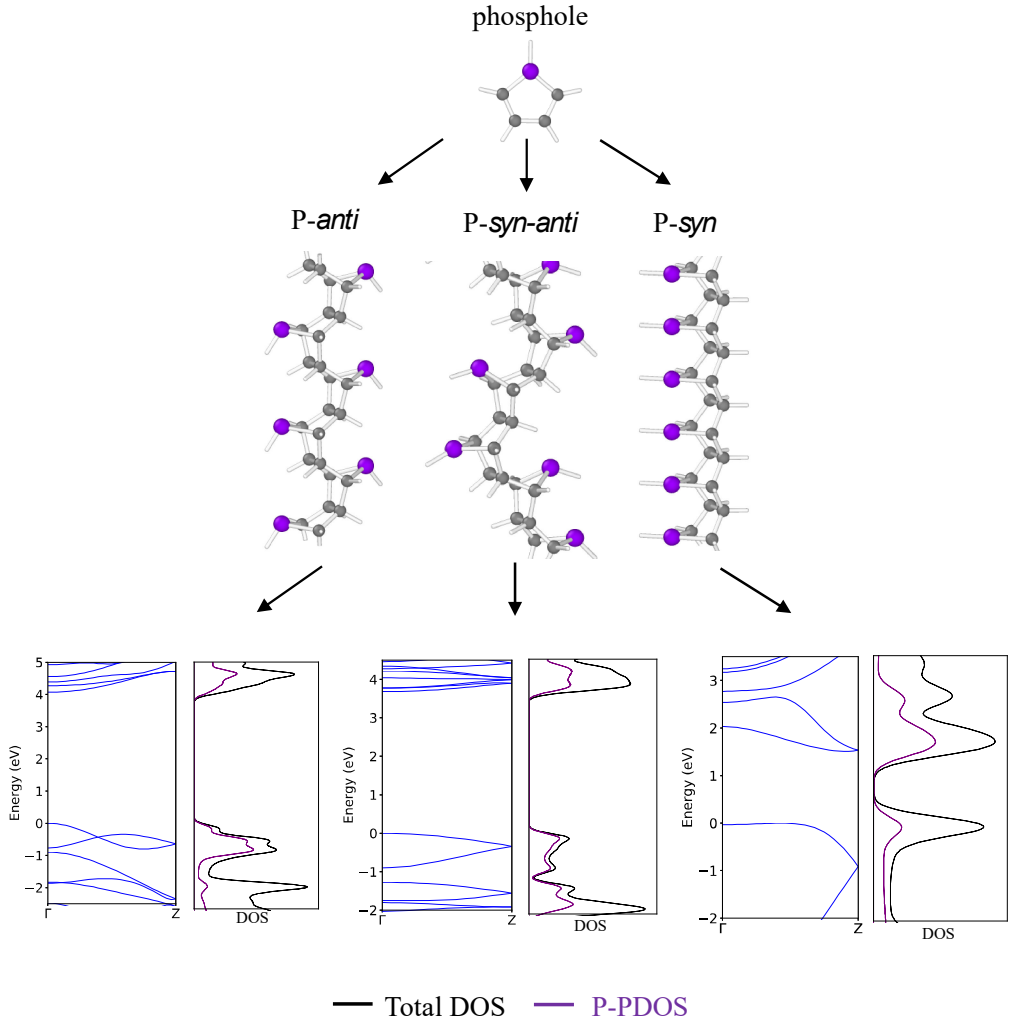

Figure S1. Structure of phosphole-derived nanothreads along with the band structures and density of states.

Deviations with respect to the expected structure were found for the *syn* material. Structural relaxation led to a distinct arrangement, containing all P atoms in a planar geometry (all of its bonds in the same plane, two being with C and one with H, as shown in Figure S1). This is due to the presence of P-H bonds aligned along the same side of the chain, which are too volumous to accomodate out-of-plane hydrogen atoms. If the H atoms were out-of-plane, in a tetrahedral geometry as in the *anti* structure, they would be as close to the neighboring P as they are to the P they are bonded to, which would require a second bond. Such deviations were not observed for the *anti* and the *syn-anti* structures, which followed the expected trend seen for other cases, due to the fact that, in these configurations, P-H groups in neighboring units are disposed on opposite sides.

Additionally to the band structures and densities of states presented in Figure S1, Table S1 shows the properties of phosphole nanothreads concerning binding energy (as defined in the main text), band gap (estimated with both GGA/PBE and hybrid HSE/DFT), and 1D Young's Modulus (in force units, as explained in the main text). All properties follow the same trends already discussed in the main text. The only particular behavior of phosphole-derived nanothreads is that their binding energies are much lower than those of the other investigated structures. This is due not only to their stability, but also to the instability of the precursor molecule. However, quantifying both contributions is beyond the scope of this work; and future investigations might consider other formation pathways, possibly involving the formation of more stable dimers.

	P-*anti*	**P-*syn-anti***	**P-*syn***
Binding Energy (eV)	-1.639	-1.592	-0.935
Band Gap GGA/PBE (eV)	4.06	3.68	1.52
Band Gap HSE (eV)	5.11	4.65	2.20
1D Young's Modulus (nN)	50.9	34.5	110.8

Table S1. Properties of phosphole-derived nanothreads.

1.2. Use of other methods for van der Waals corrections

We have performed additional calculations for the binding energy and band gap of all studied nanothreads, using two extra van der Waals correction methods available in the Quantum Espresso software: besides Grimme's D2 correction, we used theTkatchenko-Scheffler (TS) and Grimme's D3. The results are summarized in the Table below:

Nanothread	Binding Energy (eV)			Band Gap (eV)		
	D2	TS	D3	D2	TS	D3
N-anti	-0.285	-0.118	-0.082	3.65	3.49	3.65
N-syn	-0.337	-0.182	-0.162	2.90	2.79	2.90
N-syn-anti	-0.393	-0.236	-0.201	3.36	3.23	3.35
O-anti	-0.784	-0.640	-0.617	4.47	4.30	4.47
O-syn	-0.625	-0.505	-0.491	3.32	3.23	3.33
O-syn-anti	-0.783	-0.655	-0.628	4.16	4.04	4.17
S-anti	-0.461	-0.337	-0.310	3.61	3.57	3.61
S-syn	0.516	0.624	0.642	0.87	0.70	0.87
S-syn-anti	-0.437	-0.325	-0.291	2.92	2.89	2.92

Table S2. Binding energy and electronic band gap (according to GGA/PBE DFT) of all studied nanothreads according to different van der Waals corrections: Grimme's D2, Tkatchenko-Scheffler (TS), and Grimme's D3. Binding energy is defined in the main text of the paper.

From a quantitative point of view, the binding energies computed using the three corrections are different (but in the same order of magnitude), and the electronic band gaps are essentially the same. But most importantly, from a qualitative point of view, the same trends are observed when comparing different isomers for a given heteroatom or different heteroatoms for a given isomer.

1.3. Ab-initio molecular dynamics at finite temperature

We also investigated the thermal stability of selected nanothreads at room temperature (all *anti* structures and the least stable S-*syn* configuration). For that purpose, we have carried out ab-initio molecular dynamics (MD) simulations at 300K for time intervals as high as 20 ps, using an integration timestep of 1.0 fs and employing the same settings of the other DFT calculations to maintain consistency (as described in Sec. 2 of the main text). Equilibration is achieved , and no bond breaking or structural changes were observed for the *anti* structures and S-*syn* nanothread in such simulations. Curves of potential energy as function of time from MD simulations are shown in Figure S2.

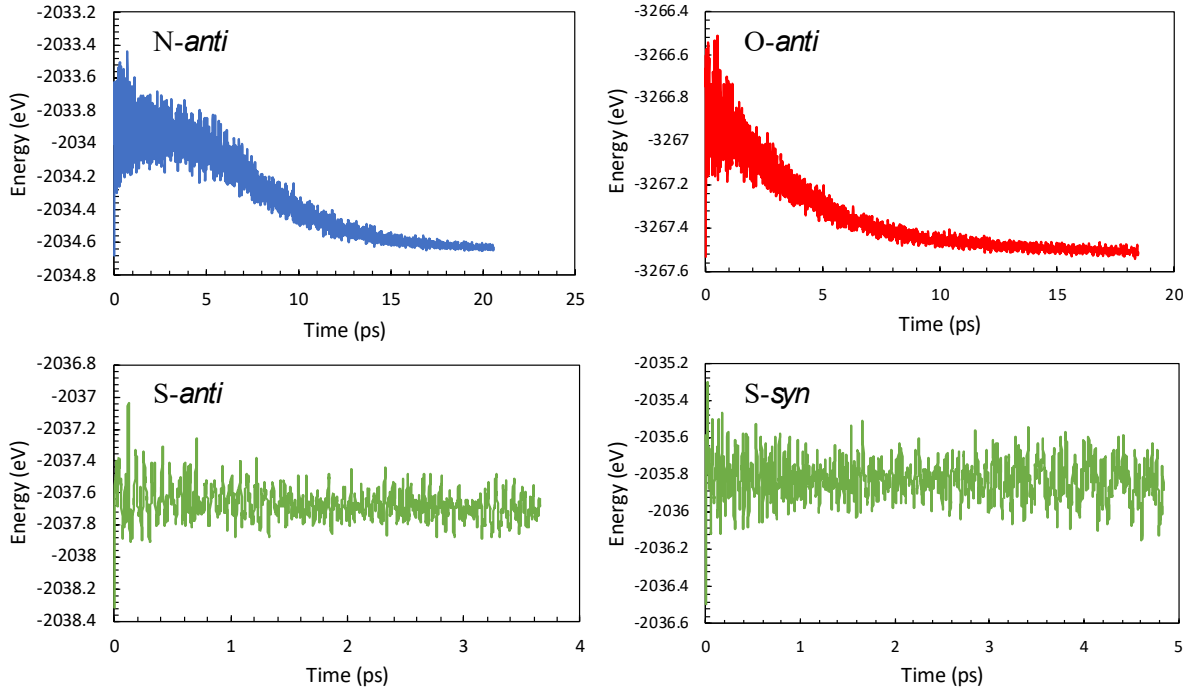

Figure S2. Potential energy of selected nanothreads as function of time during ab-initio MD simulations at 300K.

2. Nanothread atomic structures

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3. References

[1] C. Charrier, H. Bonnard, G. De Lauzon and F. Mathey, Journalof the American Chemical Society, 1983,105, 6871–6877.
[2] S. Huss, S. Wu, B. Chen, T. Wang, M. Gerthoffer, R. Hoffmann,V. Crespi, J. Badding and E. Elacqua, 2020.
[3] A. Biswas, M. D. Ward, T. Wang, L. Zhu, H.-T. Huang, J. V.Badding, V. H. Crespi and T. A. Strobel, The journal of physicalchemistry letters, 2019,10, 7164–7171.