### ELECTRONIC SUPPLEMENTARY INFORMATION

## FOR

# FUNCTIONALIZED DIAMOND NANOTHREADS FROM

## **BENZENE DERIVATIVES**

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**Topics:** 

- **S1.** More on DFT calculations convergence study
- **S2.** More on DFT calculations predicted bond lengths
- **S3.** More on DOS computation pyridine-based DNTs

### **S1.** More on DFT calculations – convergence study

DFT calculations were carried using GGA/PBE, PAW pseudopotentials from the Quantum Espresso database, a plane wave energy cutoff of 45Ry and a gamma centered  $1 \times 1 \times 18$  k-points mesh. These parameters were chosen from a convergence study. For example, Figure S1 show the dependence of the energy, forces and stress (tau\_zz) with the energy cutoff for one selected DNT configuration (strained from its equilibrium

configuration along z-direction); from these plots, we selected the value of 45 Ry for our calculations.



Figure S1. Dependence of energy, stress and forces with energy cutoff for a strained DNT configuration.

### S2. More on DFT calculations – predicted bond lengths

The C-C interatomic distances were measured for all functionalized DNT configurations used in our study. The results are summarized in Table S1, and show that the presence of the attached functional groups leads to slight changes in the  $sp^3$  C-C bond length along the nanothread. To avoid an extensive list of computed bond lengths, we provide in the table a range (minimum to maximum) of the computed values for

each configuration. More details can be taken from the atomic coordinates files, also available as Supplementary Material in a separate file.

	Bond Length Range (A)				
Configuration	CH3	NH2	ОН	F	Pyr
(1,2)	1.575 - 1.577	1.567 - 1.576	1.558 - 1.572	1.563 - 1.582	1.521 - 1.557
(1,3)	1.574 - 1.578	1.569 - 1.575	1.560 - 1.571	1.563 - 1.580	1.510 - 1.571
(1,4)	1.577 - 1.578	1.570 - 1.574	1.560 - 1.570	1.564 - 1.578	1.510 - 1.555
(1,2,3,4)	1.550 - 1.609	1.552 - 1.595	1.555 - 1.581	1.566 - 1.587	1.493 - 1.568
(1,4,2,5)	1.569 - 1.599	1.560 - 1.590	1.558 - 1.581	1.566 - 1.586	1.493 - 1.568
(1,2,3,4,5,6)	1.552 - 1.606	1.553 - 1.599	1.557 - 1.579	1.568 - 1.578	1.487 - 1.566
(1,4,2,5,3,6)	1.549 - 1.605	1.552 - 1.600	1.553 - 1.583	1.566 - 1.586	1.493 - 1.563
pristine	1.566				

Table S1. Computed C-C bond lengths for the investigated configurations.

## S3. More on DOS computation – pyridine-based DNTs

Figure S2 depicts the total electronic density of states and the orbital projected density of states for the pristine DNT and a pyridine-based DNT, namely the (1:4):pyr configuration. By comparing the plots, we can see the presence of additional states near the valence band edge of the (1:4):pyr compared to the pristine DNT, that are mainly attributed to the presence of the N heteroatoms. These additional states are closer in energy to the conduction band, leading to a reduction in the gap for the pyridine-based DNT compared to the pristine case.



Figure S2. Projected density of states (pDOS) for (a) pristine DNT and (b) pyridinebased (1,4):pyr DNT, showing the contribution of C, H and N atoms to the total density of states. The contribution of all orbitals for a given element is summed up to give the complete contribution of the atoms for each element.