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# Role of Water in Directing Diphenylalanine Assembly into Nanotubes and Nanowires **

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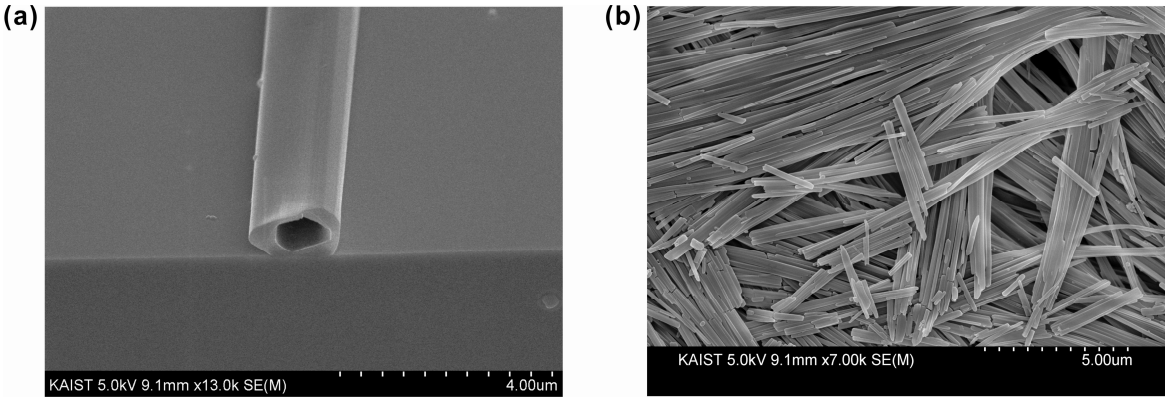


***Figure S1.*** SEM images showing the morphology of NTs (*left*) and NWs (*right*) converted from as-synthesized NWs and NTs, respectively. a) The NT morphology prepared by sonication and annealing of dried NWs in a medium of deionized water. b) The NW morphology prepared by dissolving of dried NTs in an acidic TFA solution followed by titration with $NH_4OH$.

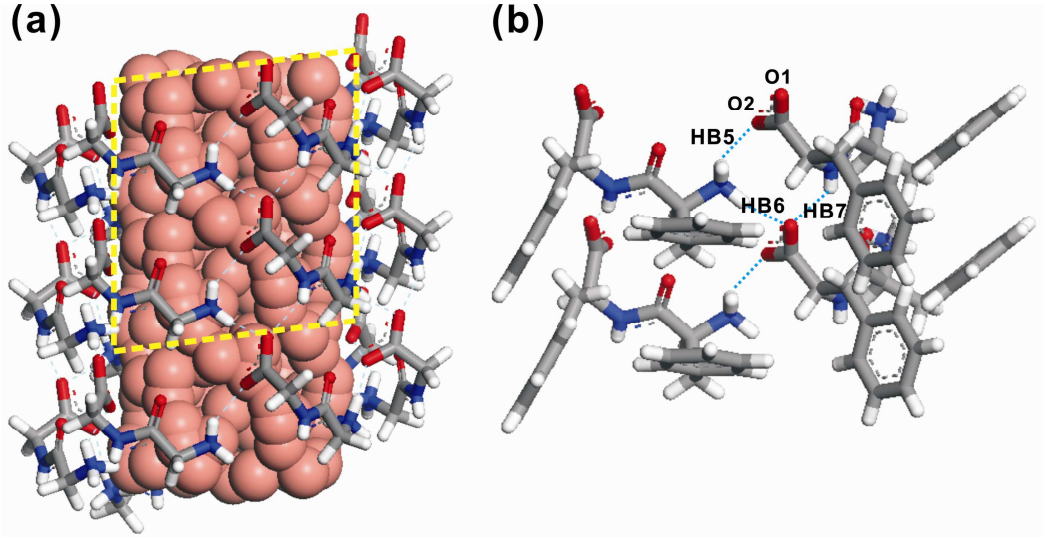


***Figure S2.*** The helical architecture around clusters of central water molecules and intermolecular hydrogen bonding networks (dotted blue lines). a) Helical architecture of the NTs. Phenyl moieties are omitted from the side chain for clarity. Light red spheres represent the water molecules of arbitrary size, in which hydrogen atoms have been omitted. b) Illustration of the intermolecular hydrogen bonds between the diphenylalanine molecules in the NTs. Three major interactions are shown as 'HB5' (*intra*-layer), 'HB6' and 'HB7' (*inter*-layer). The *intra*-layer (HB5) hydrogen bond in the NWs is weakened relative to that in the NTs (Table S2).

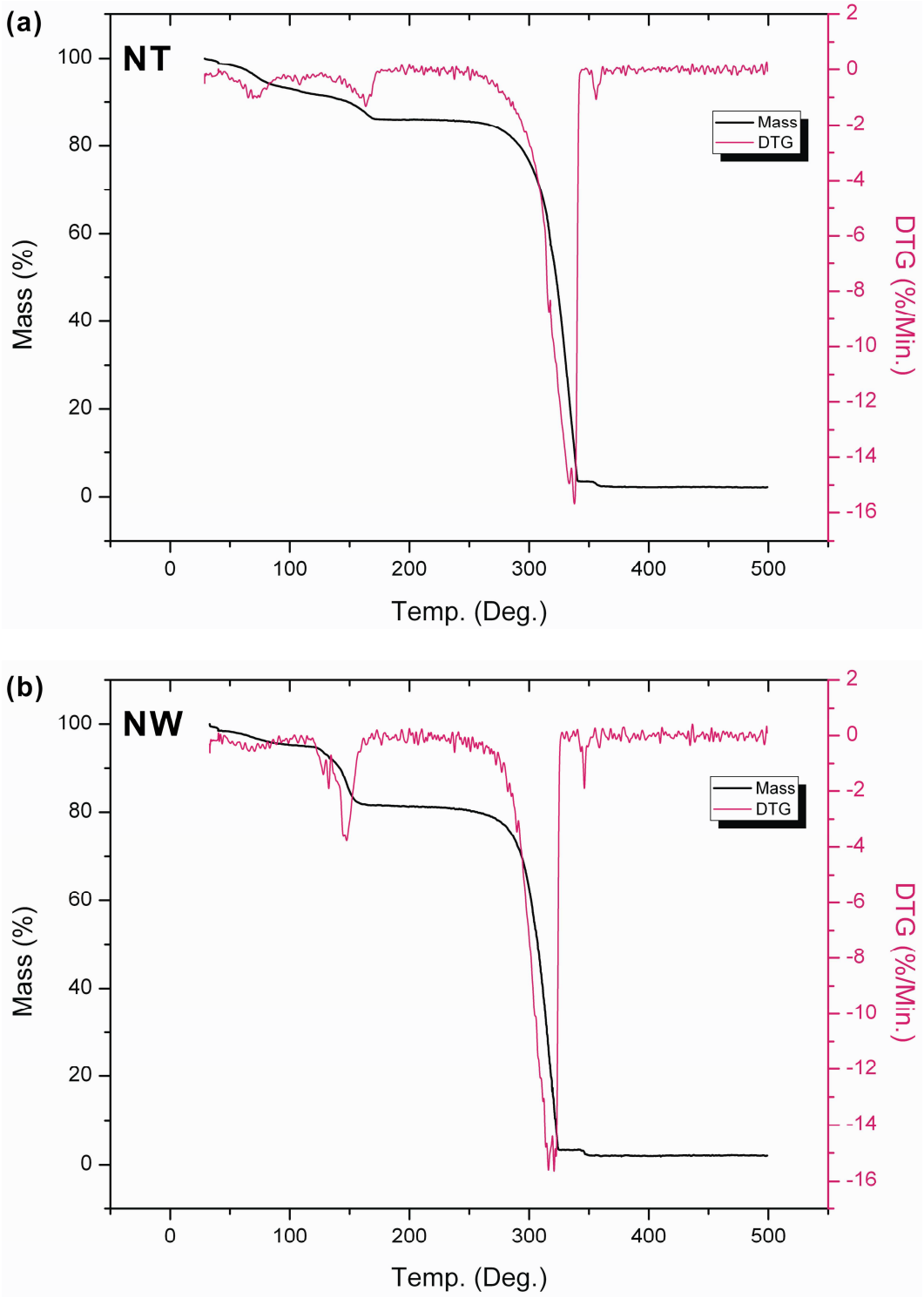


**Figure S3.** Thermo-gravimetric analysis for a) NTs and b) NWs. TGA data show a weight loss in the NT and NW sample around 611 K and 594 K, respectively, attributed to the heat-induced loss of the diphenylalanine moieties.

***Table S1***. Structural parameters and results from Rietveld refinement and experimental condition for data collection.

| | NTs | NWs |
|---|---|---|
| Mol. Formula | $C_{18}H_{20}N_2O_3 \cdot 2.76H_2O$ | $C_{18}H_{20}N_2O_3 \cdot 2.22H_2O$ |
| M. W. | 362.09 | 352.36 |
| Crystal System | Hexagonal | Hexagonal |
| Space Group (No.) | $P6_1$ (169) | $P6_1$ (169) |
| Z | 6 | 6 |
| *a* [Å] | 24.11940(18) | 24.17278(30) |
| *b* [Å] | 24.11940(18) | 24.17278(30) |
| *c* [Å] | 5.45925(6) | 5.45398(7) |
| $\alpha$ [°] | 90.0 | 90.0 |
| $\beta$ [°] | 90.0 | 90.0 |
| $\gamma$ [°] | 120.0 | 120.0 |
| V [Å$^3$] | 2750.40(4) | 2759.93(6) |
| D [g cm$^{-3}$] | 1.312 | 1.272 |
| Wavelength [Å] | 1.5489 | 1.5489 |
| Temperature [K] | 300 | 300 |
| Radiation Type | Synchrotron | Synchrotron |
| Range 2$\theta$ [°] | 2 - 70 | 2 - 70 |
| Step width 2$\theta$ [°] | 0.02 | 0.02 |
| No. of data points (N) | 3401 | 3401 |
| No. of variables (P) | 110 | 110 |
| $R_P$ | 6.00 | 6.19 |
| $R_{WP}$ | 8.33 | 8.43 |
| $R_e$ | 3.47 | 4.34 |
| $\chi^2$ | 5.76 | 3.77 |

***Table S2***. Selected intermolecular hydrogen bonding distances between the diphenylalanine-water cluster and diphenylalanine-diphenylalanine pairs (Values for intermolecular hydrogen bonding distances are given in Å).

| | Crystal Structure | NTs | NWs | Difference (NWs – NTs) |
|---|---|---|---|---|
| O1F···H-N2 (HB1) | 1.889 | 1.876 | 2.265 | 0.389 |
| O1H···H-N2 (HB2) | 2.145 | 2.184 | 2.771 | 0.587 |
| O1G···H-N2 (HB3) | 2.071 | 2.088 | 2.394 | 0.252 |
| O1E···H-N2 (HB4) | 2.336 | 2.327 | 2.388 | 0.061 |
| O2···H-N2 (HB5) | 2.130 | 2.078 | 2.437 | 0.359 |
| O1···H-N2 (HB6) | 1.813 | 1.832 | 2.095 | 0.263 |
| O1···H-N1 (HB7) | 2.281 | 2.152 | 2.347 | 0.195 |