

Supporting Information

Facile Covalent Functionalization of Boron Nitride Nanotubes via Coupling Reaction

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Supporting Table 1. Reaction optimization

| Sample | Factors change from standard condition a | Atomic % ^b | | | |
|----------|--|-----------------------|--------------|--------------|-------------|
| | | B | C | N | O |
| BNNTs | | 52.53 | 4.17 | 40.73 | 2.57 |
| 1 | H ₂ O/EtOH | 50.42 | 7.21 | 39.20 | 3.35 |
| 2 | H ₂ O | 49.34 | 7.70 | 39.22 | 3.75 |
| 3 | EtOH | 47.32 | 10.51 | 37.80 | 4.37 |
| 4 | Acetone | 49.50 | 7.41 | 39.54 | 3.55 |
| 5 | CHCl₃ | 36.01 | 20.69 | 28.22 | 6.91 |
| 6 | 200 mg salt | 47.05 | 10.24 | 38.48 | 4.23 |
| 7 | 3 days | 47.17 | 11.13 | 37.00 | 4.70 |
| 8 | 100°C | 48.00 | 9.51 | 37.22 | 5.27 |

^a: Reaction Conditions: 100 mg salt, 10 mg BNNTs, and 10 ml solvent, 18h, 55°C. ^b: Determined using XPS analysis.

Samples 1-5 were prepared using standard reaction conditions ^a. Samples 6-8 were prepared using standard reaction conditions ^a, with chloroform (CHCl₃) as the solvent and modified specific factor, as indicated in the table. 5 is an optimized sample (highlighted).

Supporting Table 2. Important IR peak

| Sample | Important peak |
|-------------|-----------------------------------|
| BNNT | 1374, 811, 795 |
| 3a | 2920, 2848, 1373, 795 |
| 3b | 2924, 2847, 1378, 803 |
| 3c | 2925, 2845, 1377, 801 |
| 3d | 2925, 2852, 1740, 1374, 798 |
| 3e | 2925, 2883, 2194, 1653, 1379, 809 |
| 3f | 2960, 1507, 1456, 1373, 940, 806 |
| 3g | 2924, 2845, 1377, 800 |

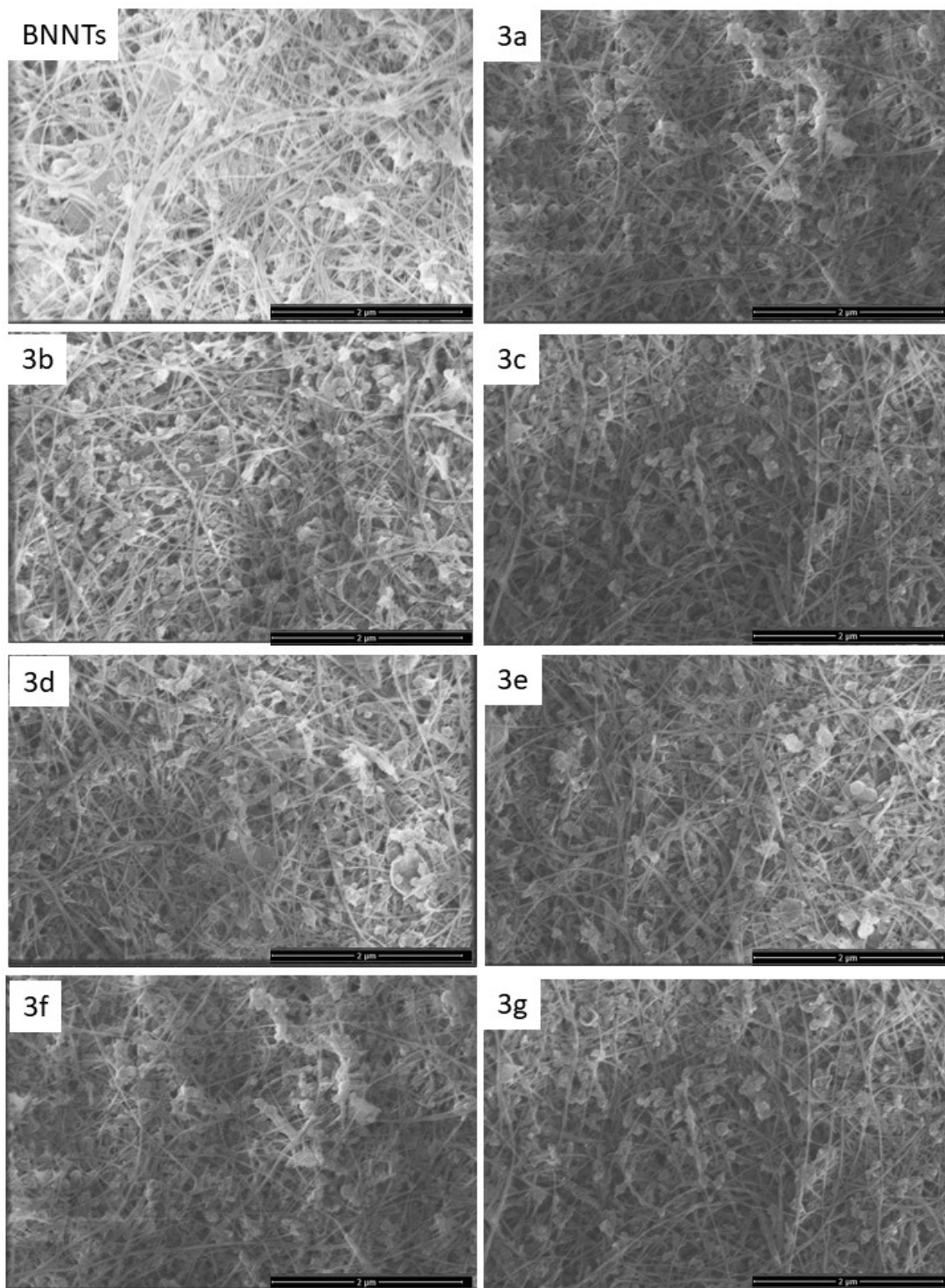
Supporting Table 3. XPS composition of BNNTs and 3a-3g

| Sample | Atomic % ^b | | | | | |
|--------------|-----------------------|-------|-------|------|------|------|
| | B | C | N | O | F | Br |
| BNNTs | 52.53 | 4.17 | 40.73 | 2.57 | | |
| 3a | 49.17 | 8.40 | 37.75 | 4.45 | | 0.22 |
| 3b | 49.03 | 8.39 | 37.64 | 4.43 | 0.51 | |
| 3c | 49.81 | 6.62 | 39.70 | 3.81 | | |
| 3d | 45.82 | 13.71 | 36.46 | 4.01 | | |
| 3e | 44.18 | 15.65 | 35.08 | 5.09 | | |
| 3f | 39.34 | 22.44 | 31.20 | 7.02 | | |
| 3g | 35.61 | 16.41 | 43.27 | 4.71 | | |

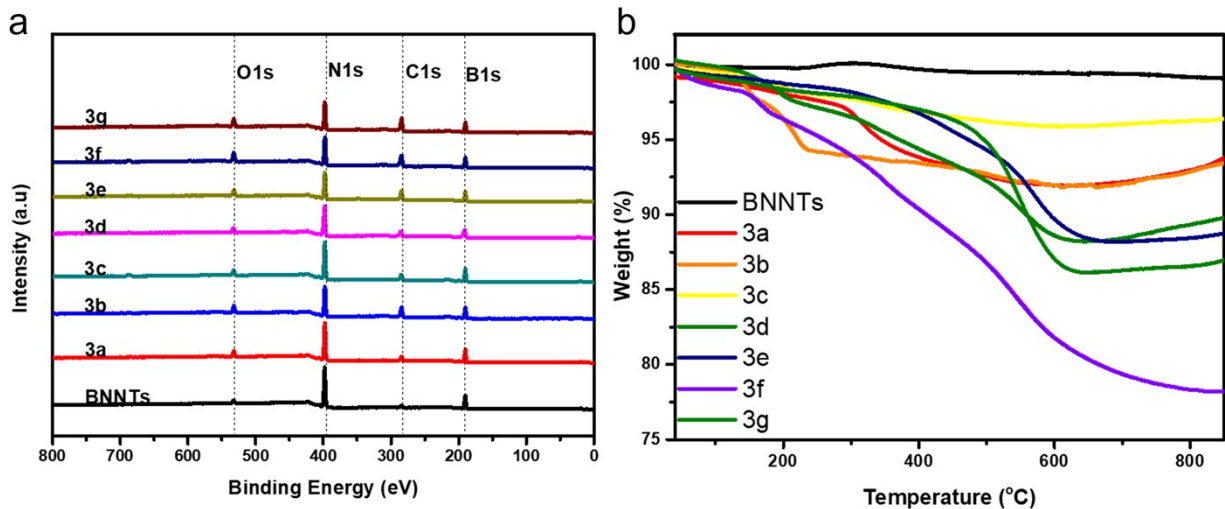
Supporting Table 4. Weight loss (%) of sample 3a – 3g

| Sample | Weight loss (%) |
|-----------|-----------------|
| 3a | 8.1 |
| 3b | 8.2 |
| 3c | 4.1 |
| 3d | 11.8 |
| 3e | 11.8 |
| 3f | 21.8 |
| 3g | 13.9 |

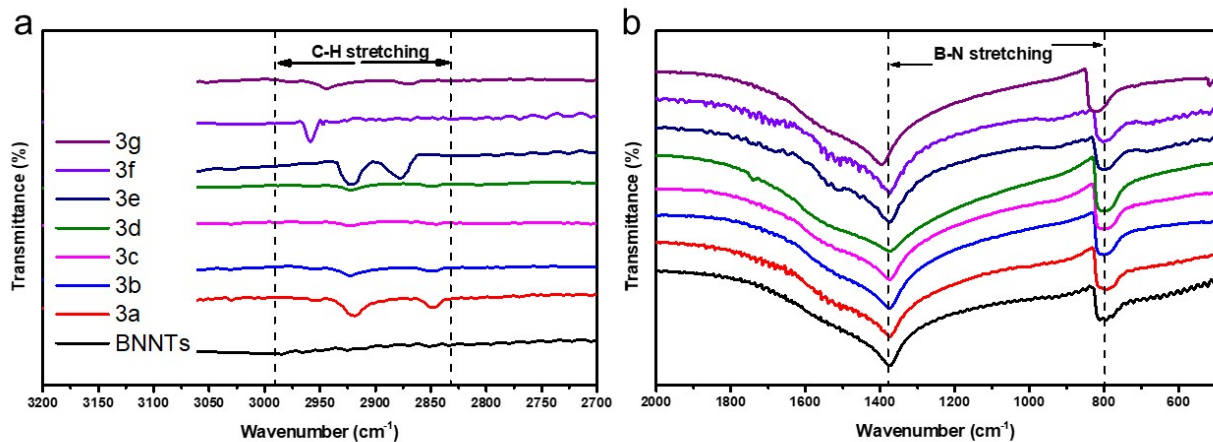
Supporting Figure 1: SEM of BNNTs, 3a-3g proved the stability of nanotubes after the reaction.



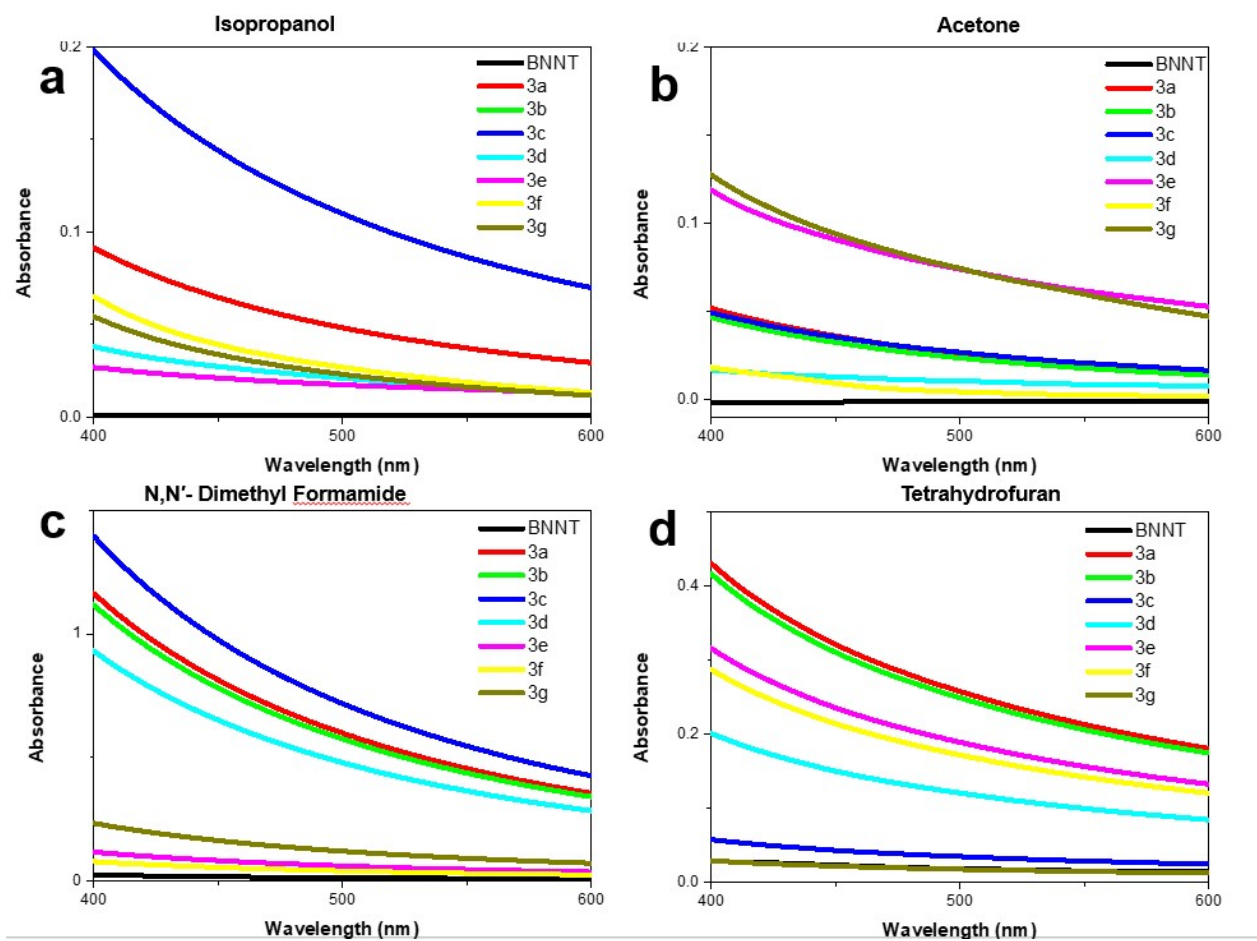
Supporting Figure 2 XPS TGA of sample 3a-3f



Supporting Figure 3 FTIR and magnified FTIR of sample 3a-3f



Supporting Figure 4, estimate dispersion by UV spectra of sample 3a-3f, procedure followed by reference¹



Reference

- (1) Lee, S.-H.; Kim, M. J.; Ahn, S.; Koh, B. Purification of Boron Nitride Nanotubes Enhances Biological Application Properties. *Int. J. Mol. Sci.* **2020**, *21* (4), 1529. <https://doi.org/10.3390/ijms21041529>.