

**Supplemental Materials for**  
**Theoretical study on  $(n, n)$ -nanotubes rolled-up from B/N**  
**substituted Me-graphene**

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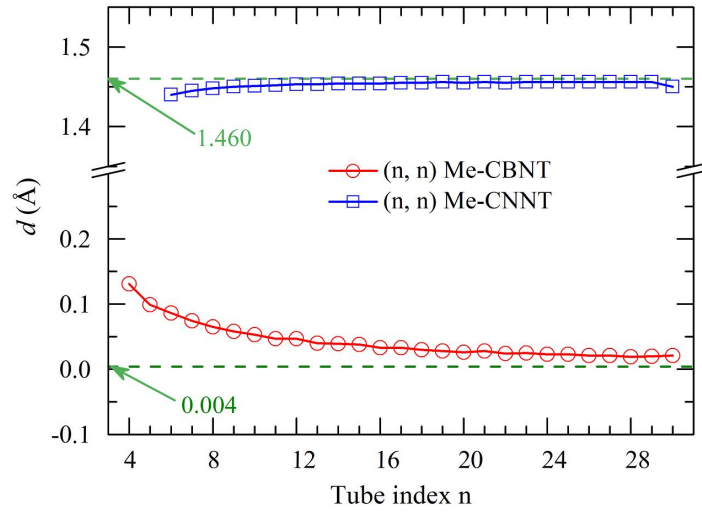
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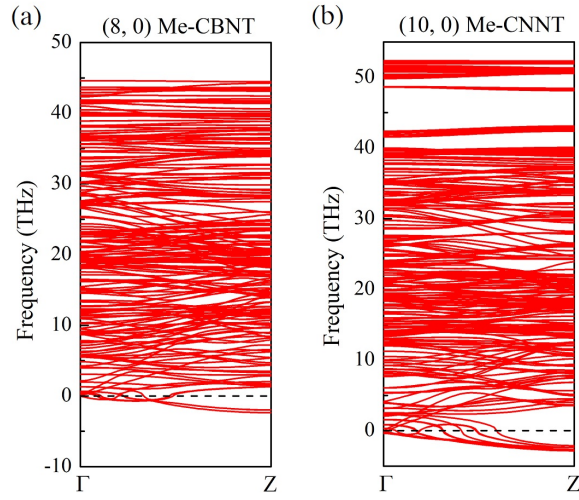
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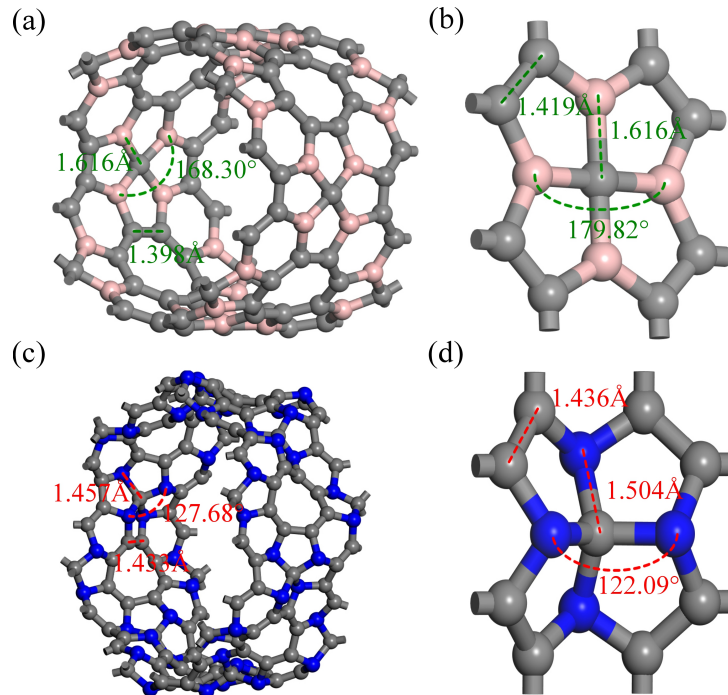
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**Figure S1** The geometric wall-thicknesses  $d$  of the  $(n, n)$  type Me-CBNT and Me-CNNT systems optimized at the PBE level. The dashed lines indicate the thicknesses of the corresponding 2D Me-C<sub>8</sub>B<sub>4</sub>C and Me-C<sub>8</sub>N<sub>4</sub>C layers.



**Figure S2** The phonon dispersion relations of (a) (8, 0) Me-CBNT and (b) (10, 0) Me-CNNT with obvious soft modes, estimated at the PBE level.



**Figure S3** The bond lengths and angles in the systems: (a) (4, 4) Me-CBNT, (b) monolayer Me-C<sub>8</sub>B<sub>4</sub>C, (c) (6, 6) Me-CNNT, and (d) Me-C<sub>8</sub>N<sub>4</sub>C.