*Supporting Information*

**Table S1.** Optimized average bond length, average bond angle, and N_atom (the number of atoms in unit cell) of $g\_C_2O$ nanosheets and $C_2O$ nanotubes.

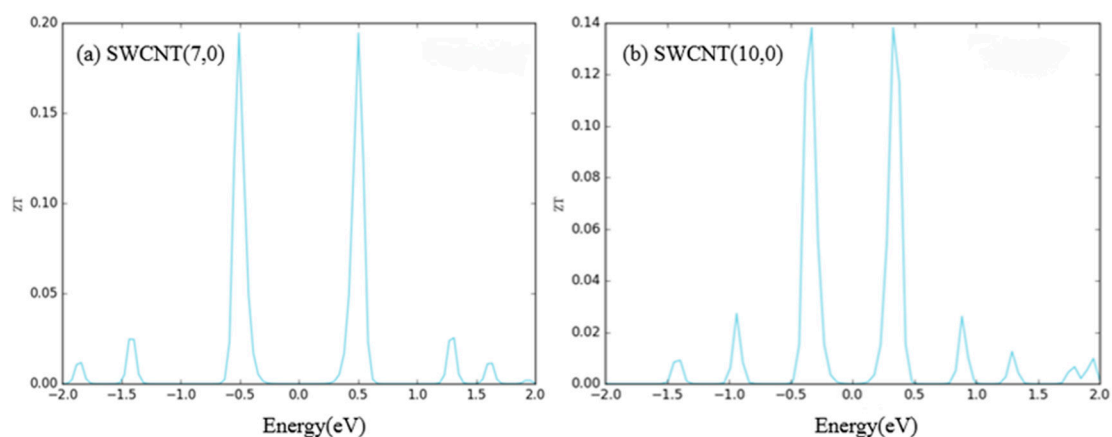|  | $g\_C_2O$ | N_atom | $D_{C\text{-}O}(\text{Å})$ | $D_{C\text{-}C}(\text{Å})$ | $A_{C\text{-}O\text{-}C}(°)$ |
|---|---|---|---|---|---|
| **Nanosheet** | (0, 0) | 18 | 1.38 | 1.39 | 115.72 |
| **Zigzag** | (4, 0) | 72 | 1.39 | 1.40 | 111.96 |
|  | (6, 0) | 108 | 1.39 | 1.40 | 113.90 |
|  | (8, 0) | 144 | 1.38 | 1.40 | 114.48 |
|  | (10, 0) | 180 | 1.38 | 1.40 | 115.24 |
|  | (12, 0) | 216 | 1.38 | 1.40 | 115.41 |
|  | (14, 0) | 256 | 1.38 | 1.40 | 115.63 |
|  | (16, 0) | 288 | 1.38 | 1.40 | 115.74 |
|  | (18, 0) | 324 | 1.38 | 1.40 | 115.79 |
| **Armchair** | (4, 4) | 72 | 1.40 | 1.40 | 110.23 |
|  | (6, 6) | 108 | 1.39 | 1.40 | 110.99 |
|  | (8, 8) | 144 | 1.39 | 1.40 | 112.67 |
|  | (10, 10) | 180 | 1.39 | 1.40 | 113.64 |
|  | (12, 12) | 216 | 1.39 | 1.40 | 113.73 |
|  | (14, 14) | 256 | 1.38 | 1.40 | 113.66 |
|  | (16, 16) | 288 | 1.38 | 1.41 | 115.54 |
|  | (18, 18) | 324 | 1.38 | 1.40 | 114.93 |



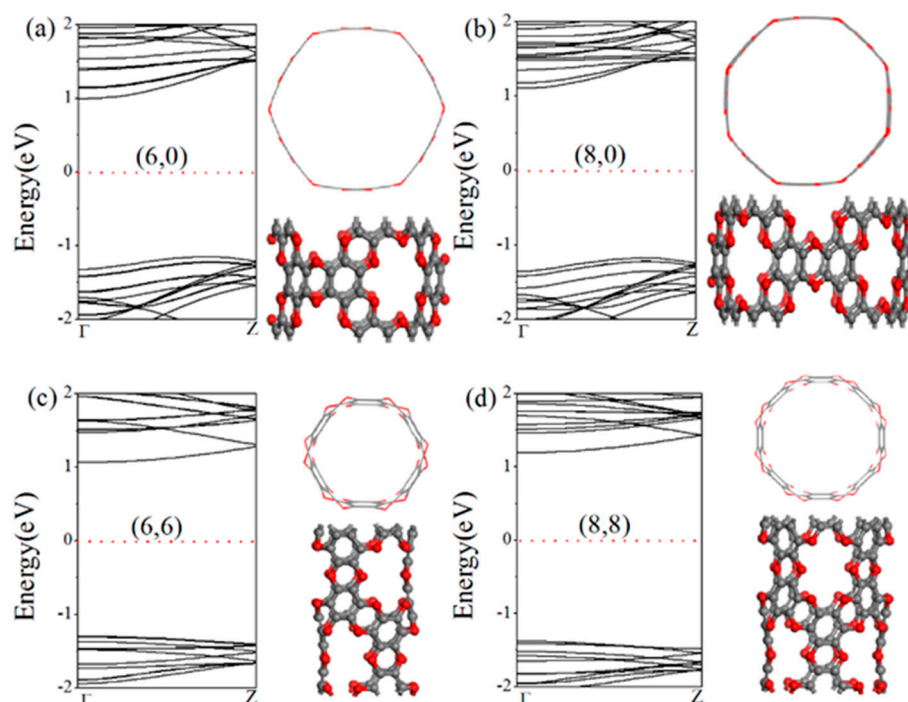**Figure S1.** ZT value at 300 K for (**a**) SWCNT(7, 0) and (**b**) SWCNT(10, 0).

**Figure S2.** The band structure of Z_C$_2$ONT and A_C$_2$ONT on the left, the top view of the linear structure, and the side view of the club structure on the right: (a) (6, 0); (b) (8, 0); (c) (6, 6); (d) (8, 8).
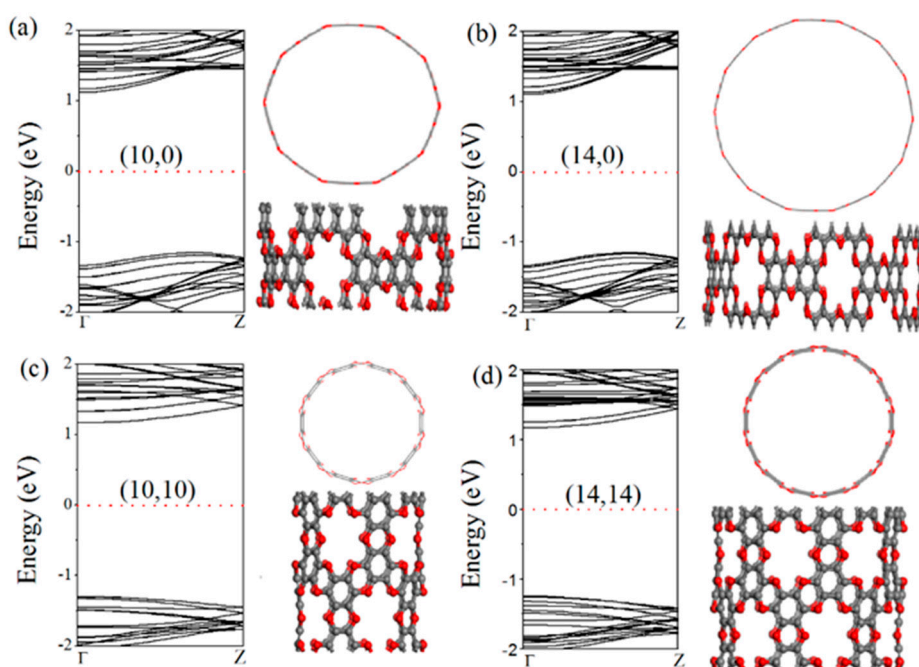


**Figure S3.** The band structure of Z_C$_2$ONT and A_C$_2$ONT on the left, the top view of the linear structure, and the side view of the club structure on the right: (a) (10, 0); (b) (14, 0); (c) (10, 10); (d) (14, 14).
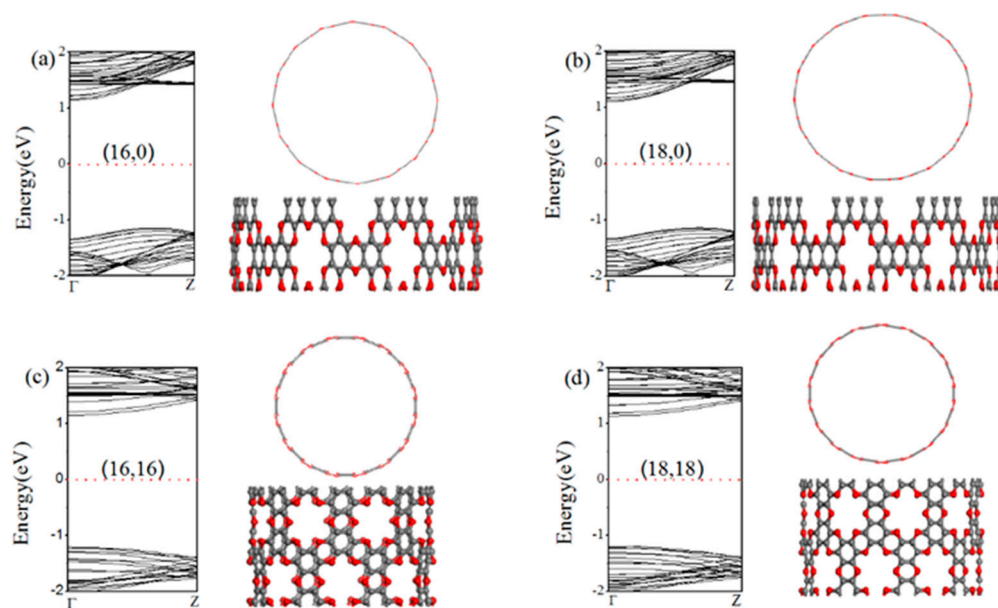
**Figure S4.** The band structure of $Z_{C_2ONTs}$ and $A_{C_2ONTs}$ on the left, the top view of the linear structure, and the side view of the club structure on the right: (a) (16, 0); (b) (18, 0); (c) (16, 16); (d) (18, 18).
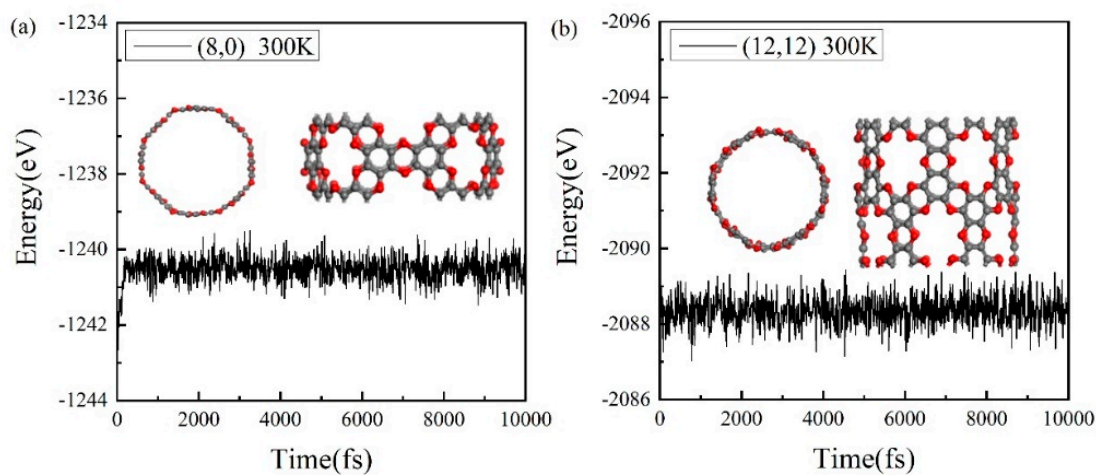


**Figure S5.** The atomic structure of $C_2ONT$ in the AIMD simulation at 300 K after the time scale of 10 ps: (**a**) $Z\_C_2ONT$ (8, 0) and (**b**) $A\_C_2ONT$ (12, 12).
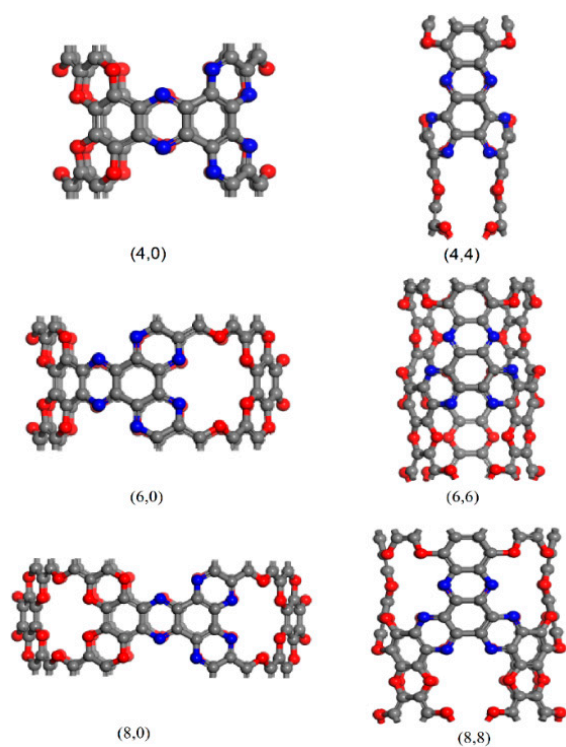
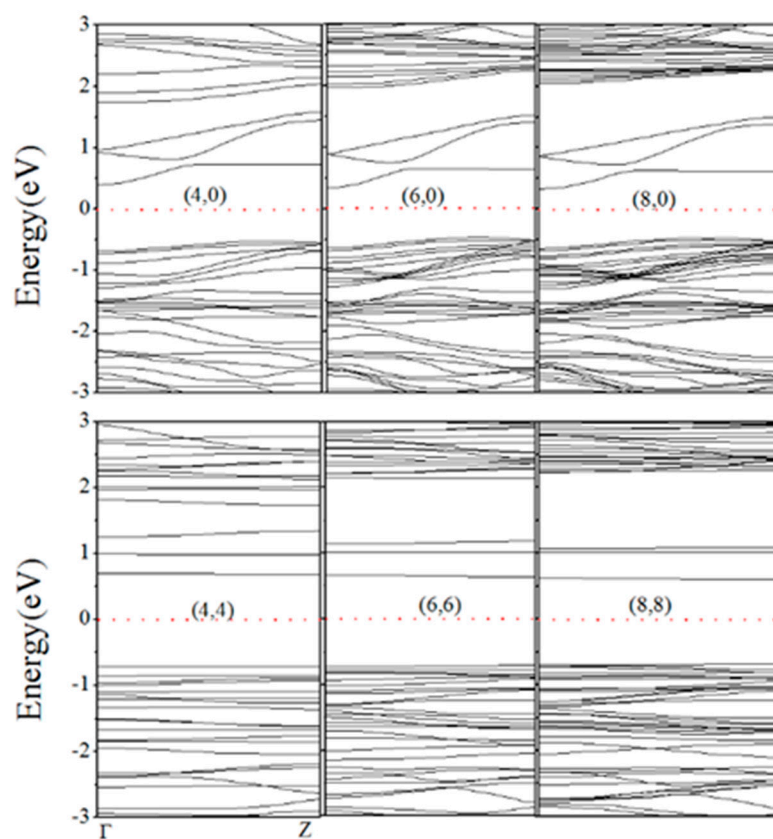**Figure S6.** The structure of $C_2ONT$ after N−doping.



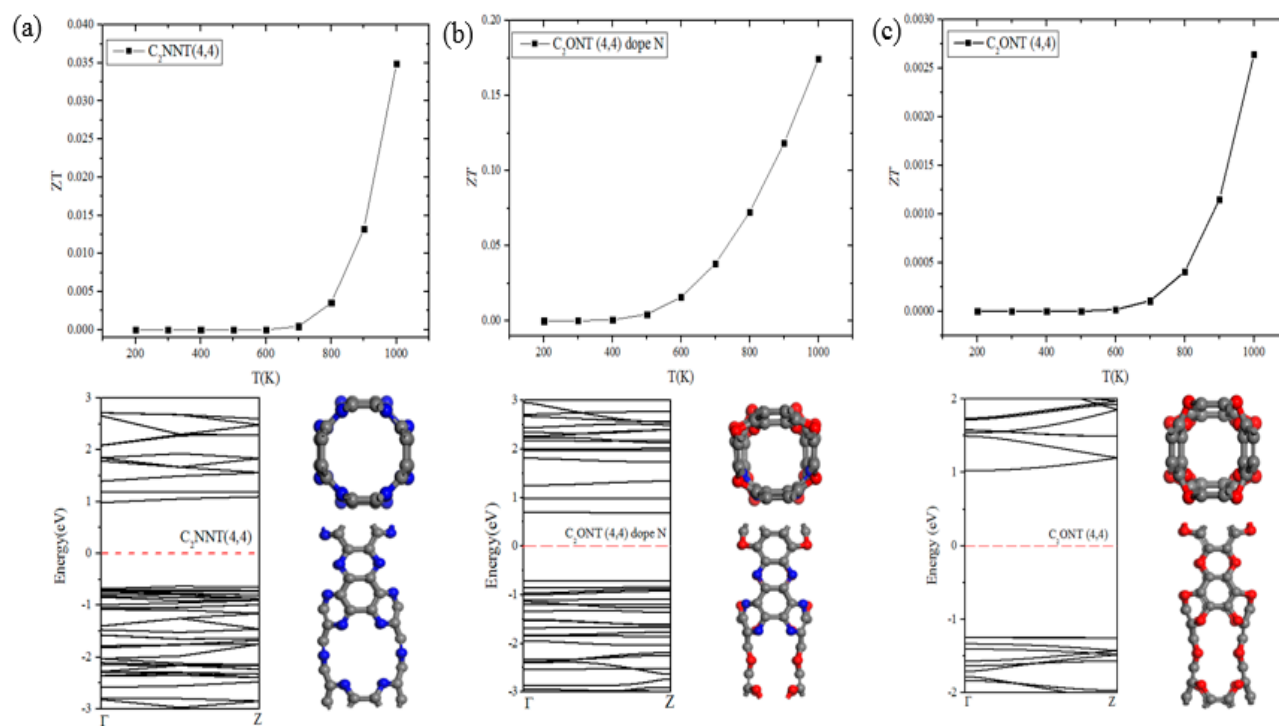**Figure S7.** The band structure of $C_2ONT$ after N−doping.

**Figure S8.** Trends in energy band structures, geometries, and ZT values of nanotubes with temperatures. (**a**) $C_2NNT$ (4, 4), (**b**) $C_2ONT$ (4, 4) doped with N, and (**c**) $C_2ONT$ (4, 4).