

Stability and Electronic Structures of Triazine-Based Carbon Nitride Nanotubes

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Figure S1. Comparison of the diameter (d) versus the chirality index n for (n,n) and $(n, 0)$ TACNNTs and CNTs. Blue and red labels in the horizontal axis represent those for armchair and zigzag tubes, respectively.

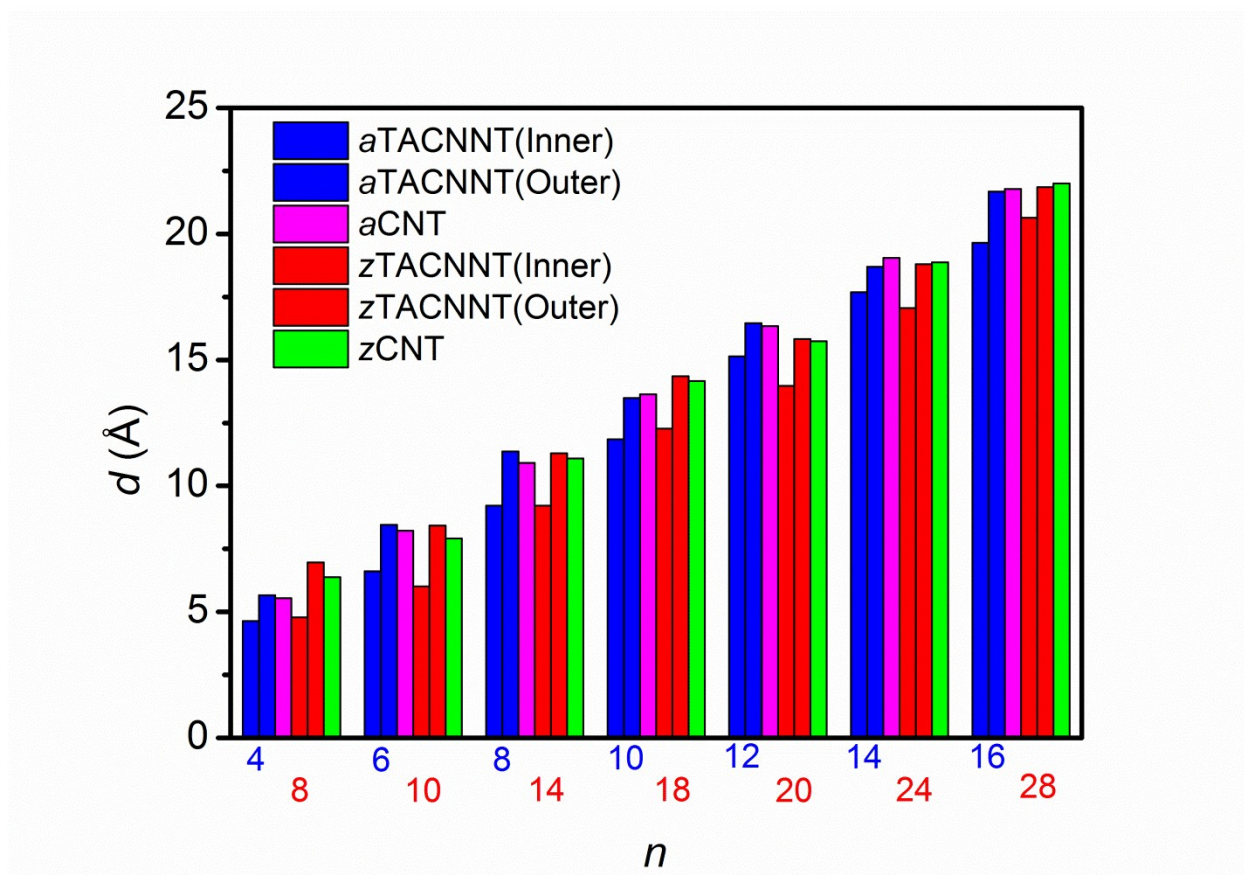
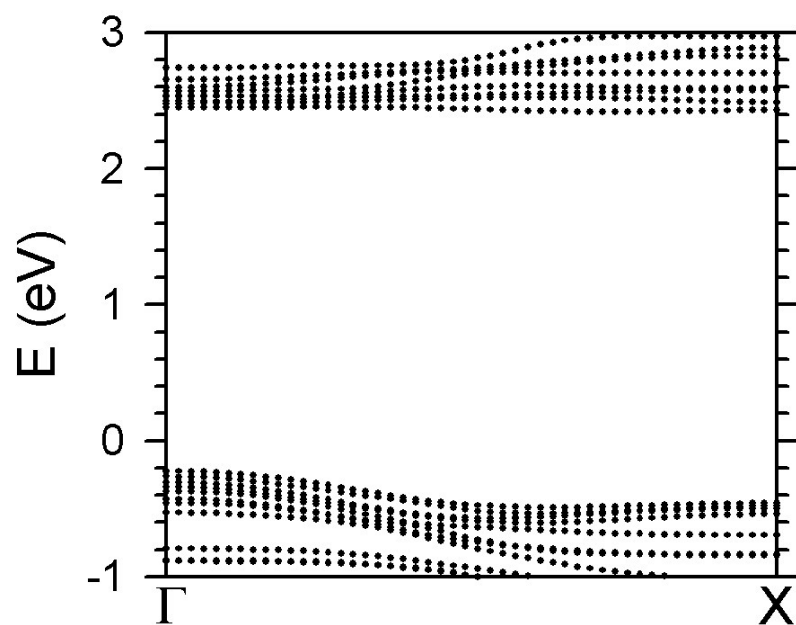


Figure S2. The band structures of (8,8) (a) and (14,14) (b) TACNNTs.

(a)



(b)

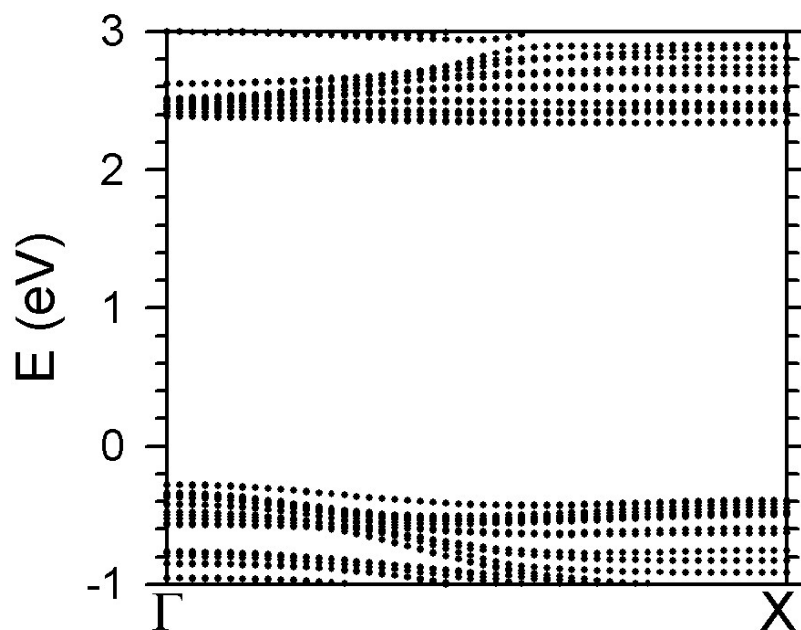
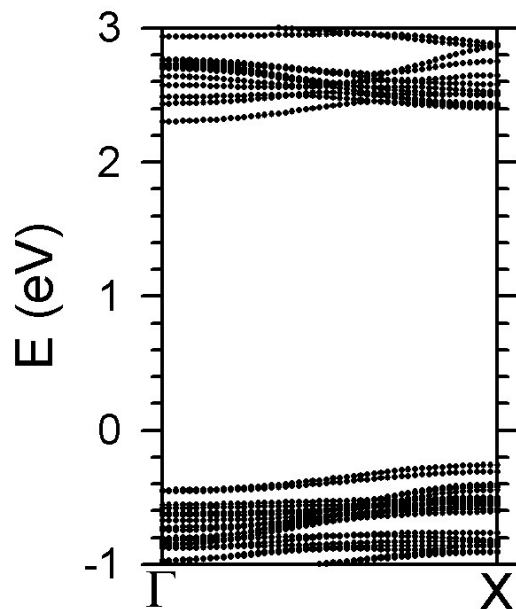


Figure S3. The band structures of P_g^- (a) and P_p^0 (b) doped (14,0) TACNNTs, where P_g and P_p^0 denote the graphitic and outward pyridinelike phosphorus atoms, respectively.

(a)



(b)

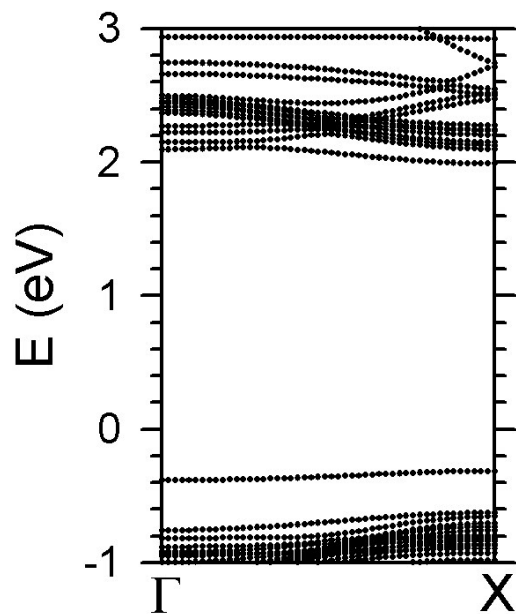
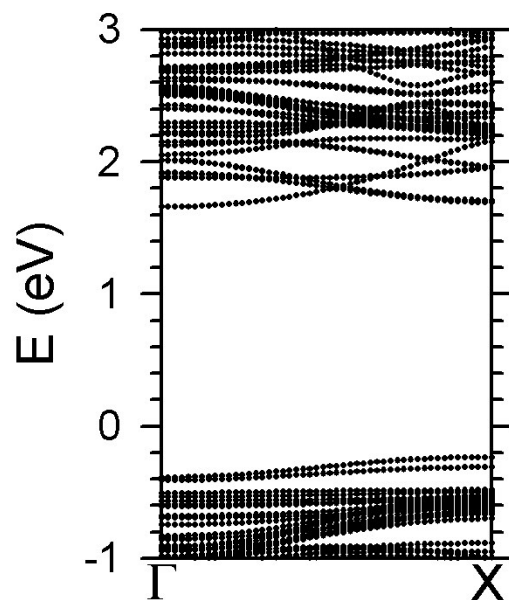


Figure S4. The band structures of FF (a) and FR (b) configurations for (10,0) $@P_g$ -(20,0) TACNNT.

(a)



(b)

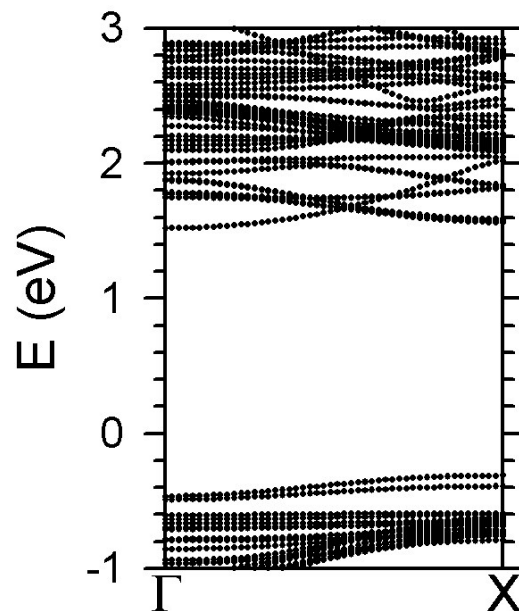
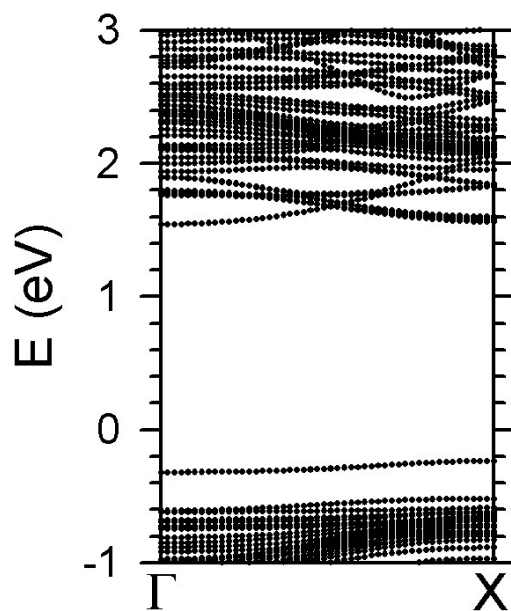


Figure S5. The band structures of FF (a) and FR (b) configurations for $(10,0)@P_p^o-(20,0)$ TACNNT.

(a)



(b)

