

Potentiality of One-dimensional blue phosphorene nanotube as a water splitting photocatalyst

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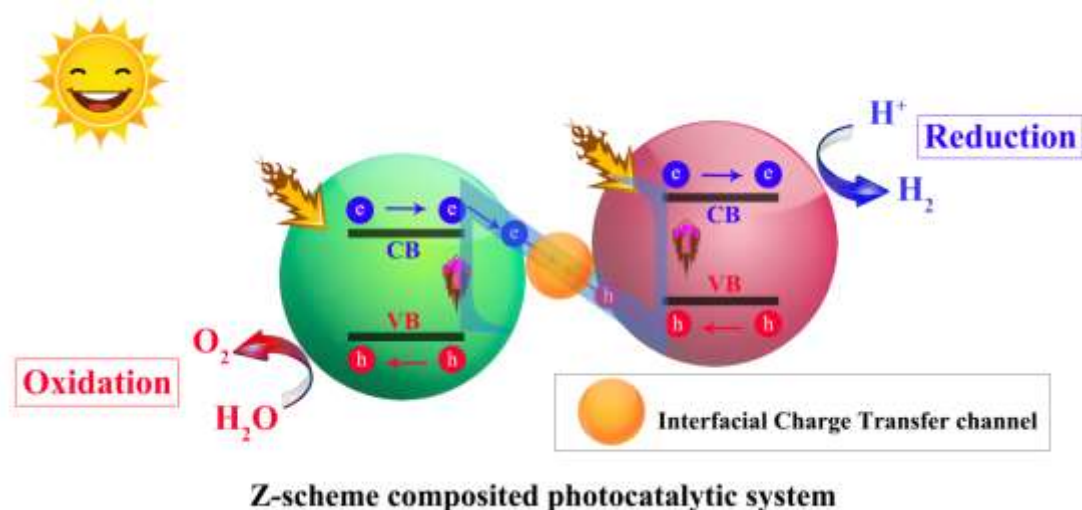


Fig. S1 The schematic illustration of Z-scheme photocatalytic system.

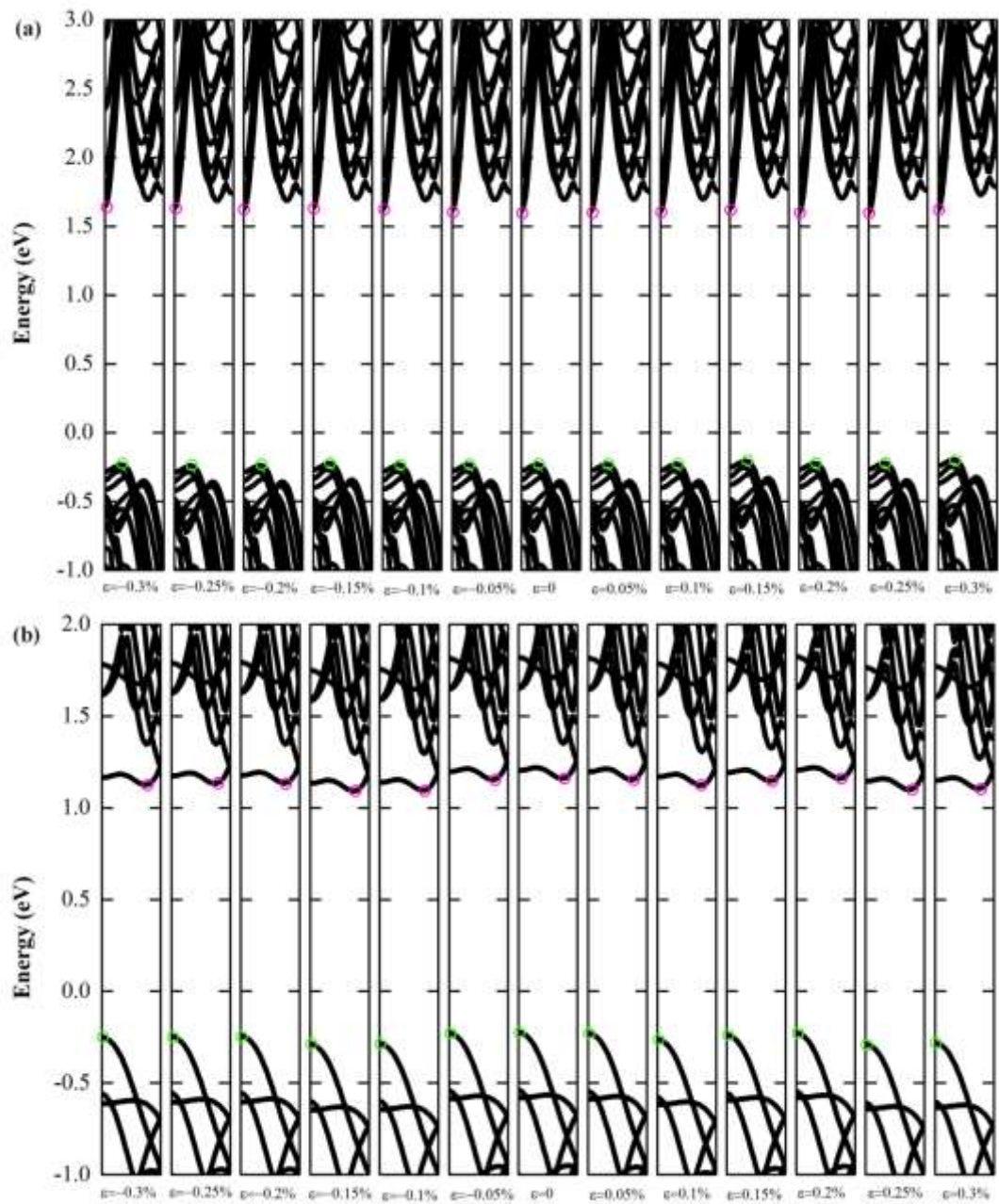


Fig. S2 The band structures of (a) (8, 8), and (b) (8, 0) BPNTs with respect to strain calculated by PBE. The VBM and CBM are marked by the green and purple circles.

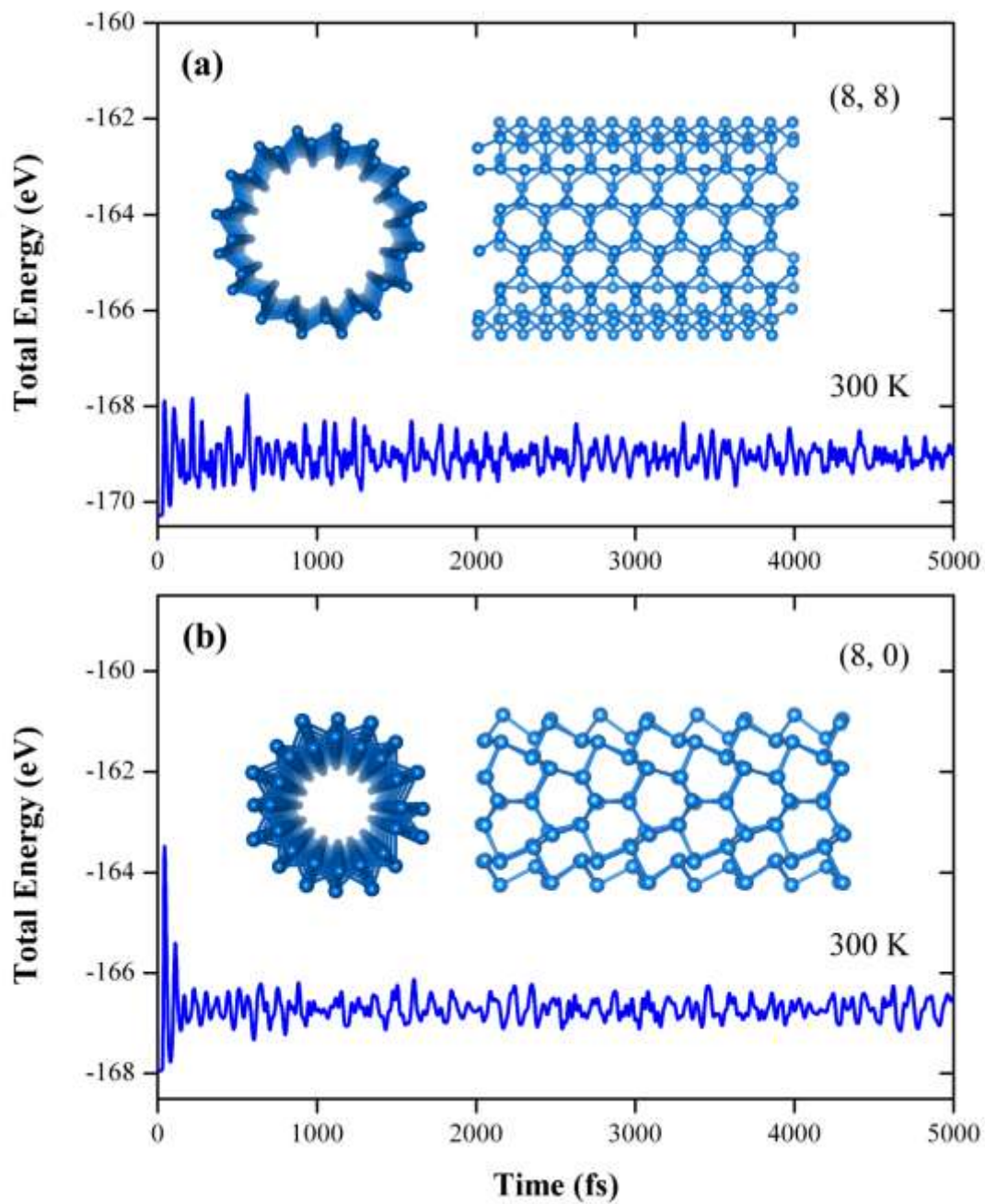


Fig. S3 AIMD simulations of (a) armchair and (b) zigzag BPNTs for 5 ps with a time step of 1 fs at 300 K.

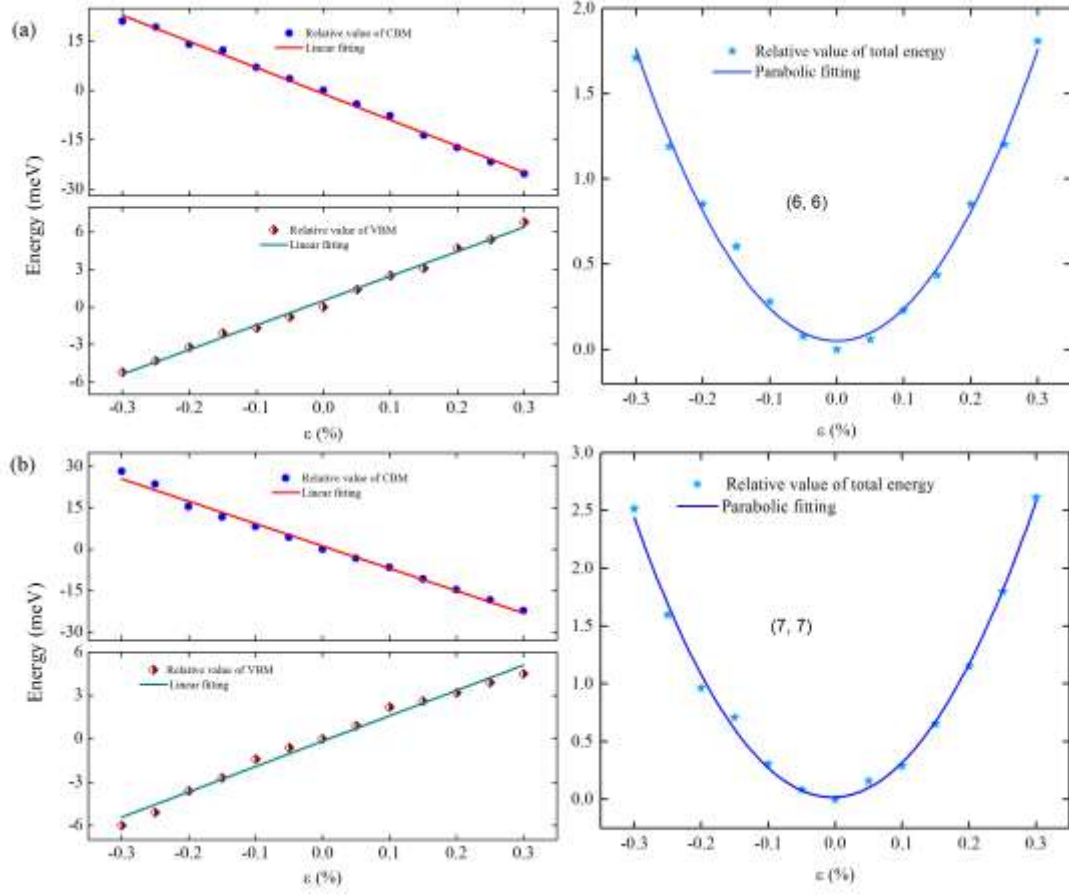


Fig. S4 The CBM, VBM, and total energy variations, as well as their corresponding fittings for (a) (6, 6), and (b) (7, 7) armchair BPNTs with respect to strain.

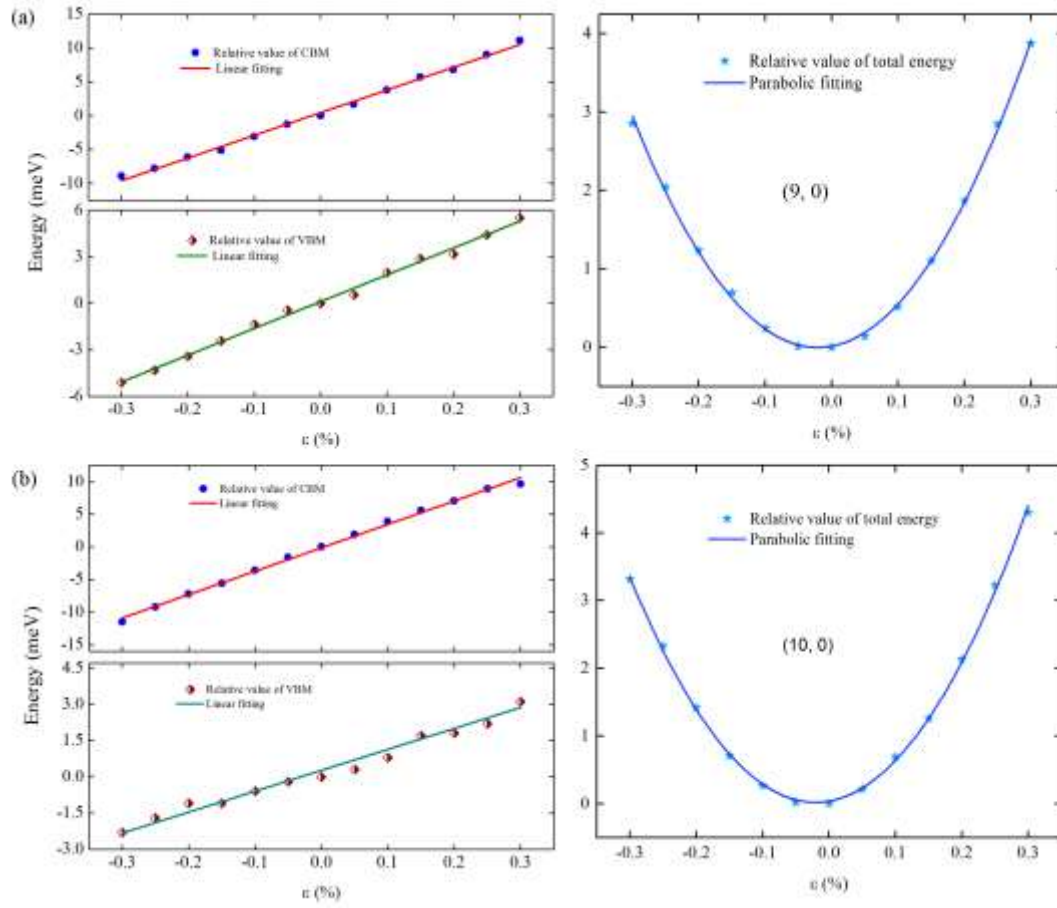


Fig. S5 The CBM, VBM, and total energy variations, as well as their corresponding fittings for (a) (9, 0), and (b) (10, 0) zigzag BPNTs with respect to strain.