Electronic supplementary information

Nanotube-Terminated Zigzag Edge of Phosphorene formed by Self-Rolling Reconstruction

Junfeng Gao, Xiangjun Liu, Gang Zhang*, and Yong-Wei Zhang*

Institute of High Performance Computing, A*STAR, Singapore 138632

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Fig. S1 The carefully energy cutoff and k-mesh test for structure relaxations. It is clearly that the energy difference is lower

than 10⁻⁴ eV/atom when energy cutoff is 400 eV. Besides, the (5×1) k-mesh for zz PNRs is good converged.



Fig. S3 The HSE06 calculated band structures of PNRs with z5 edge terminated by a nanotube. The band gap increases to 1.23 eV, which is about twice that from the standard PBE calculation. It is noted that the HSE06 calculated band arrangement is similar to PBE calculations.



Fig. S4 The perspective views of various edge structures explored in the present study.