Electronic Supplementary Material (ESI) for Nanoscale Advances.

Robust Charge Spatial Separation and Tunable Band Gap of Low-Energy Tube-Reconstructed Phosphorene Edges

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CALCULATION DETAILS

Our DFT calculations were carried out by the VASP code[1], using the planewave basis with an energy cutoff of 460 eV, the projector augmented wave pseudopotentials[2], and the generalized gradient approximation parameterized by Perdew-Burke-Ernzerhof (GGA-PBE)[3] for exchange-correlation functional. The Brillouin zones of the supercells were sampled by 10×1×1 uniform k point mesh. A 15 Å vacuum layer is provided along the non-periodic direction to prevent periodic boundary conditions from affecting the structure. With fixed cell parameters, the model structures were fully optimized using the convergence criteria of 10^{-5} eV for the electronic energy and 10^{-2} eV/Å for the forces on each atom.

Ab initio molecular dynamics (AIMD) simulations were carried out to estimate thermal stability. The AIMD simulations were performed at 300 K, and simulation time is from 5 ps to 9 ps, using NVT ensemble with the Nose´ thermostat[4] 1 fs/step.

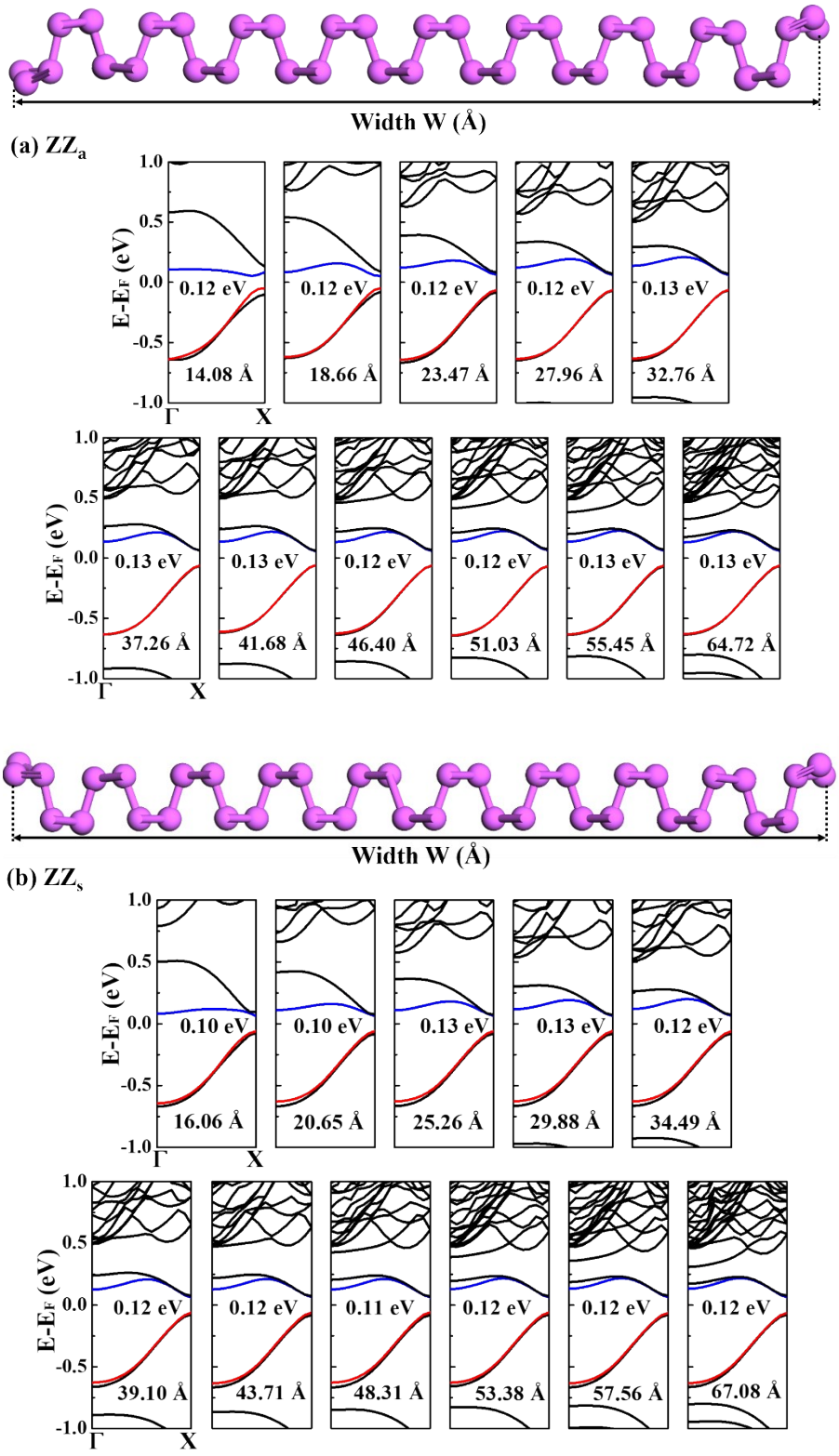

Figure S1. Band structures of ZZ PNRs with different widths with asymmetric (a) and symmetric (b) edges.

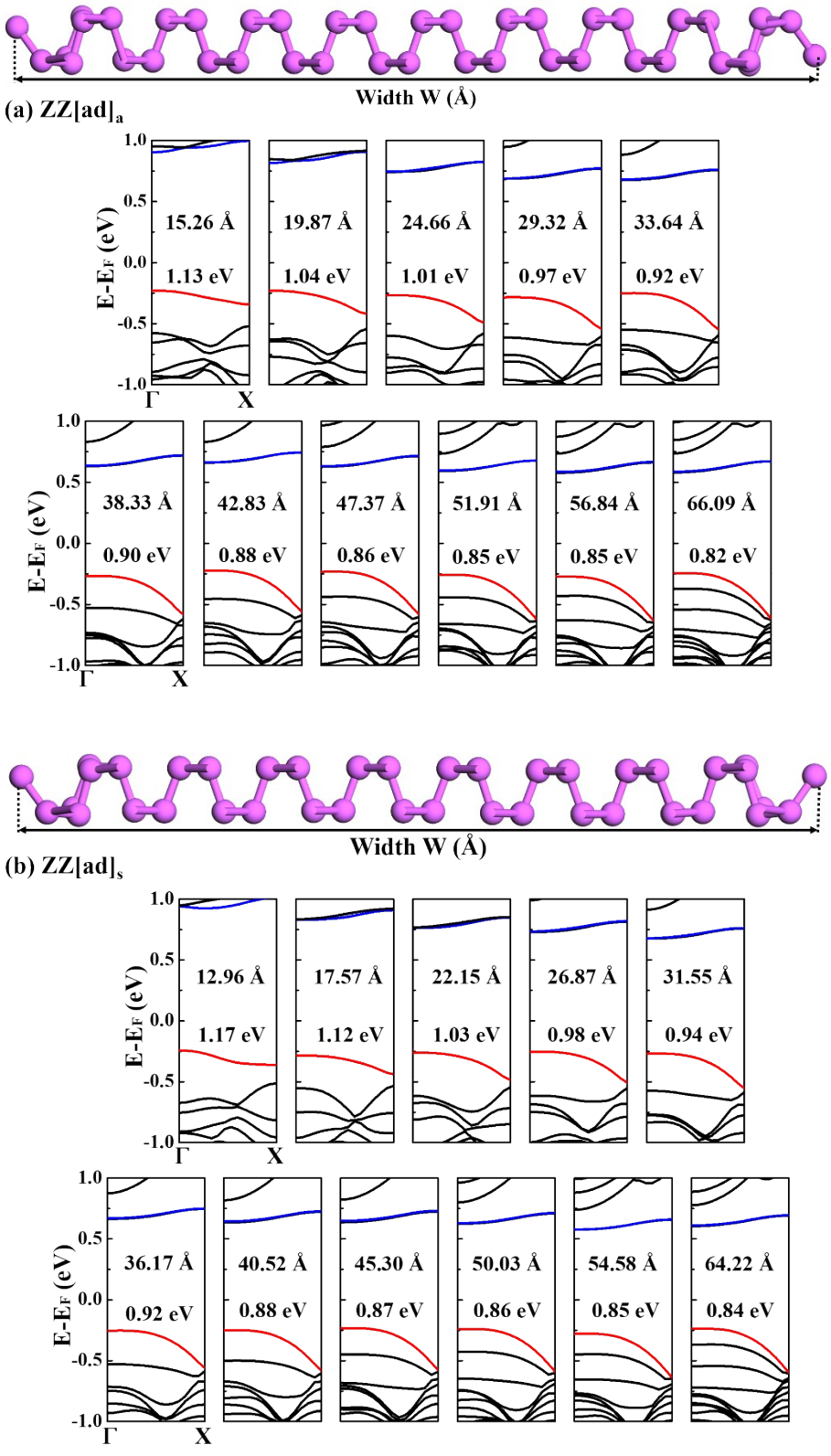

Figure S2. Band structures of ZZ[ad] PNRs with different widths with asymmetric (a) and symmetric (b) edges.

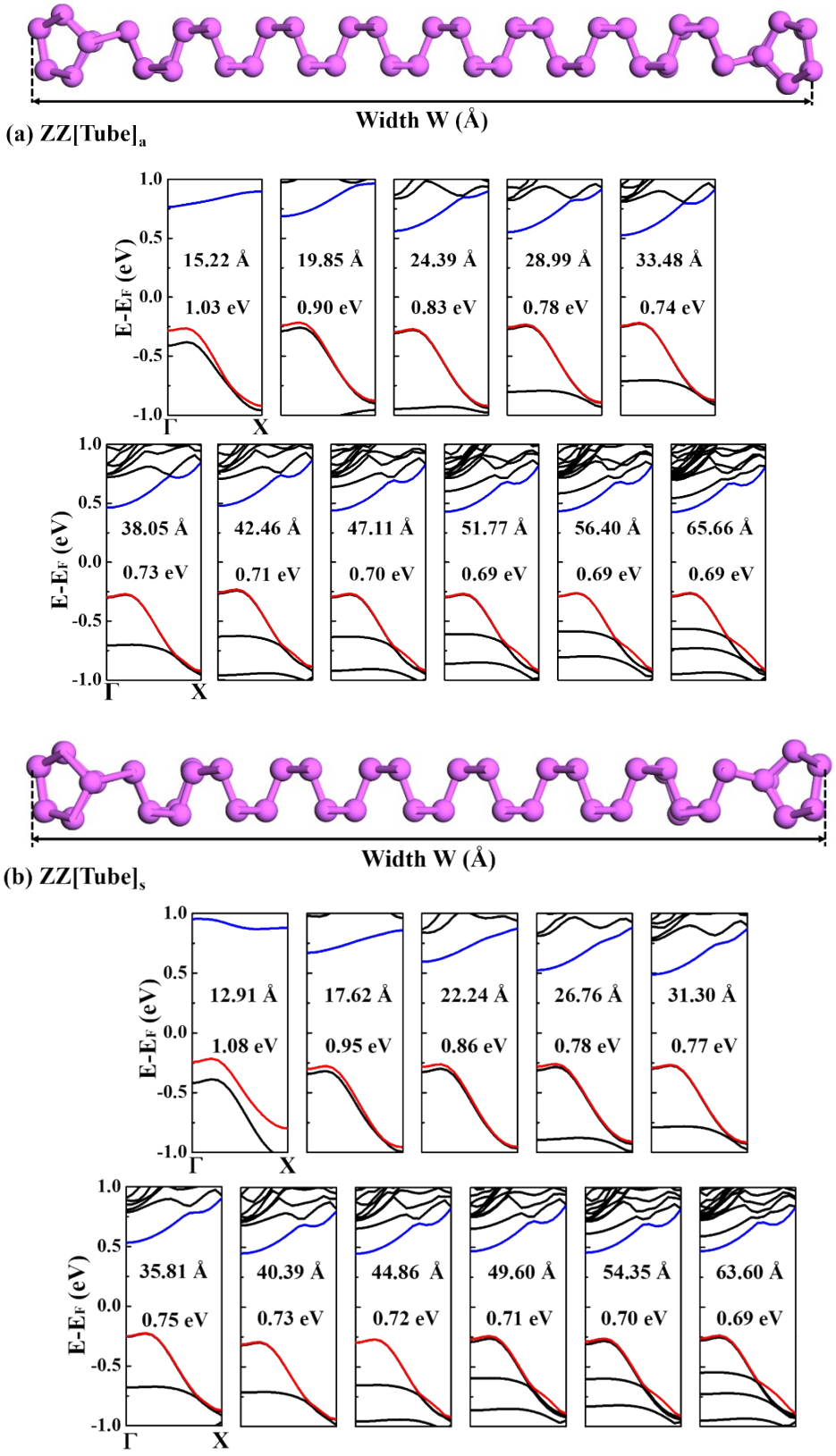

Figure S3. Band structures of ZZ[Tube] PNRs with different widths with asymmetric (a) and symmetric (b) edges.

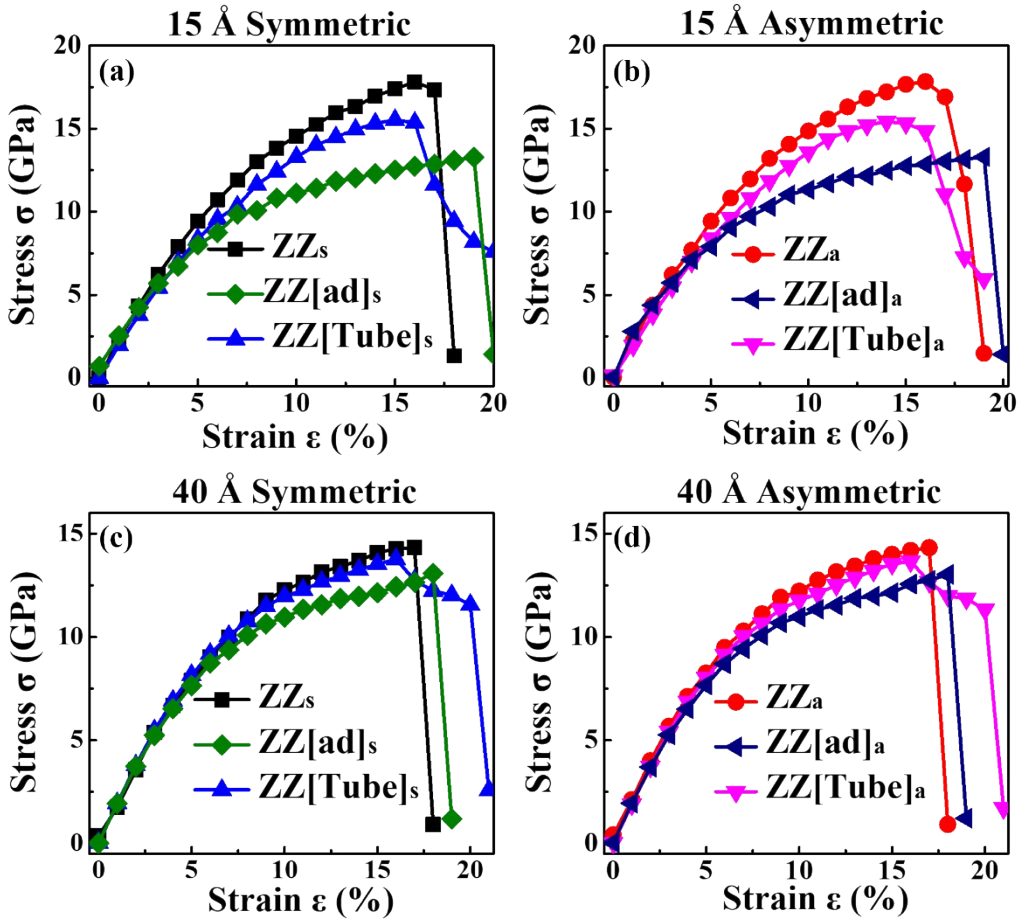

Figure S4. The stress–strain curves for ZZ, ZZ[ad] and ZZ[Tube] PNRs with either symmetric or asymmetric edges with different width.

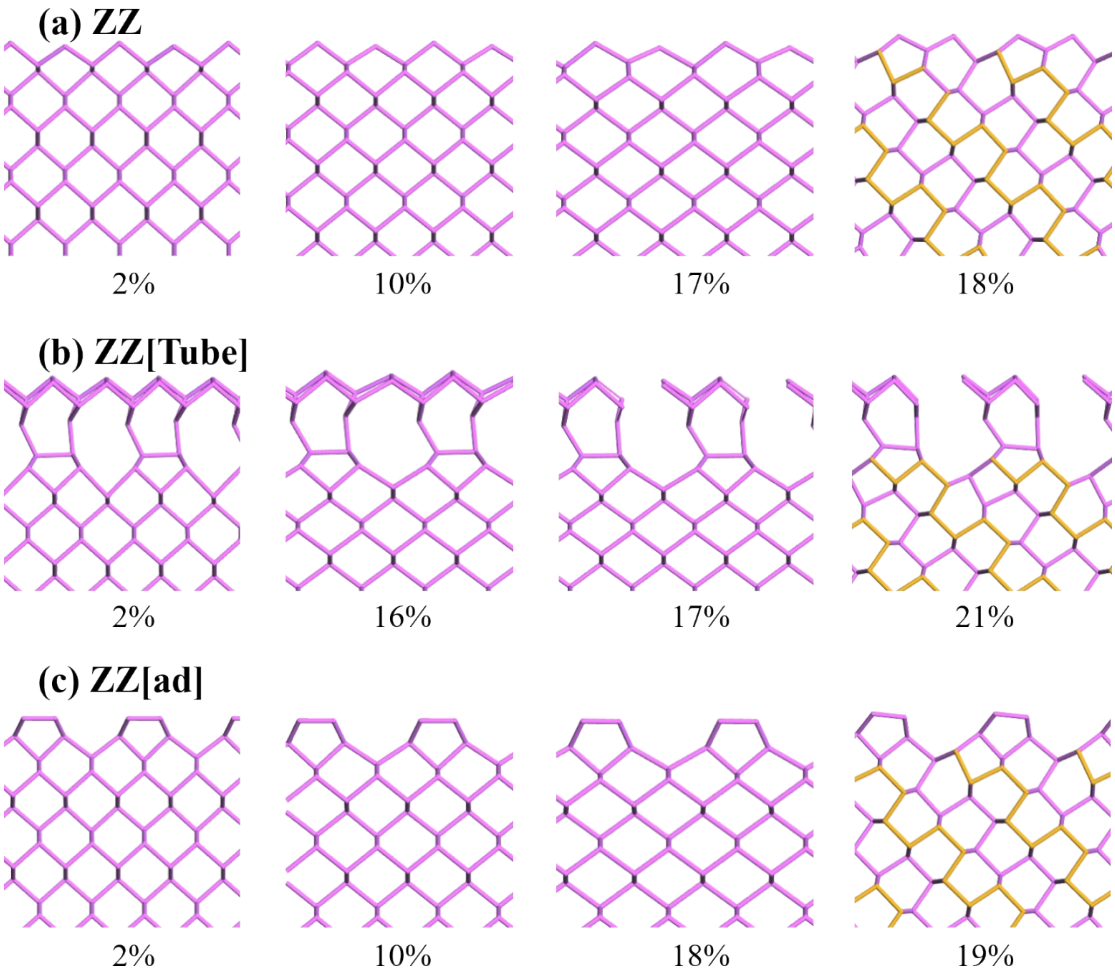

Figure S5. The structural deformation of ZZ, ZZ[Tube] and ZZ[ad] PNRs with asymmetric edges during stretching. The last column represents the failure at the critical tensile strain. The ZZ[Tube] fractured for the first time when the applied strain was 17%, and the phase transition occurred at 21%, causing the second fracture.

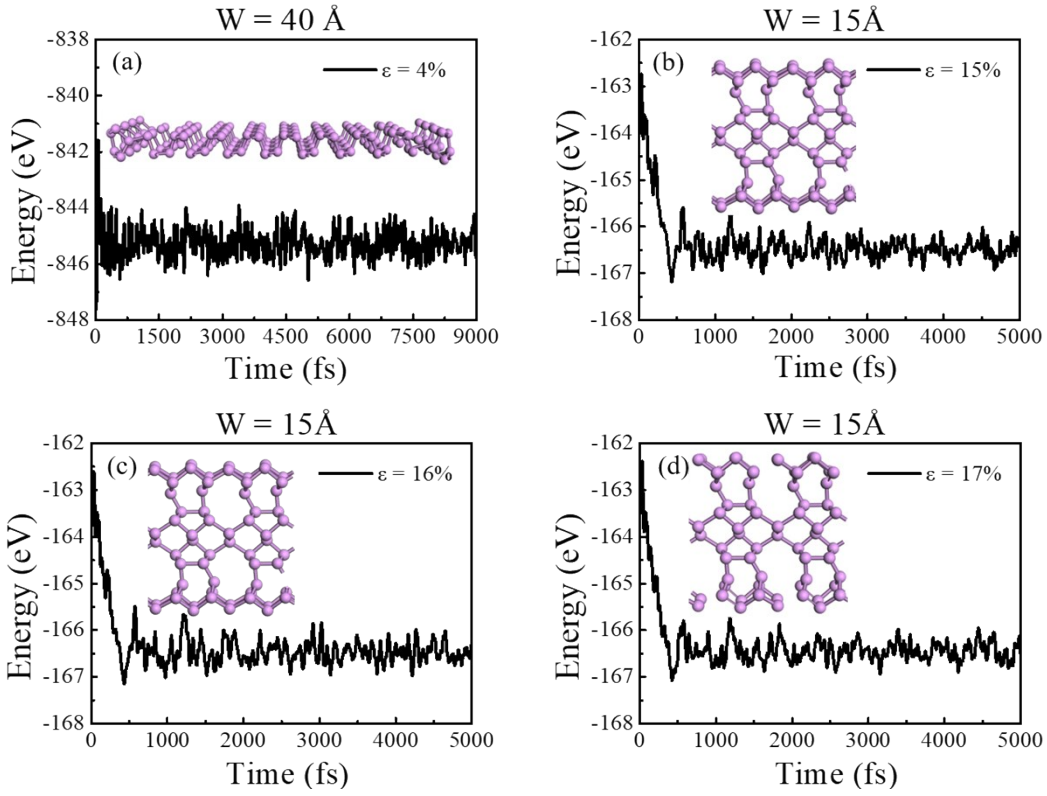

Figure S6. Equilibrated structure of the ZZ[Tube] PNRs and fluctuations of total energy as a function of simulation time in AIMD simulations at 300 K. (a)ZZ[Tube] PNRs with the width of 40Å, fluctuations of total energy as a function of simulation time under strain at 4%. (b)-(d) representing under strain at 15%, 16% and 17%, ZZ[Tube] PNRs with the width of 40Å, fluctuations of total energy as a function of simulation time.

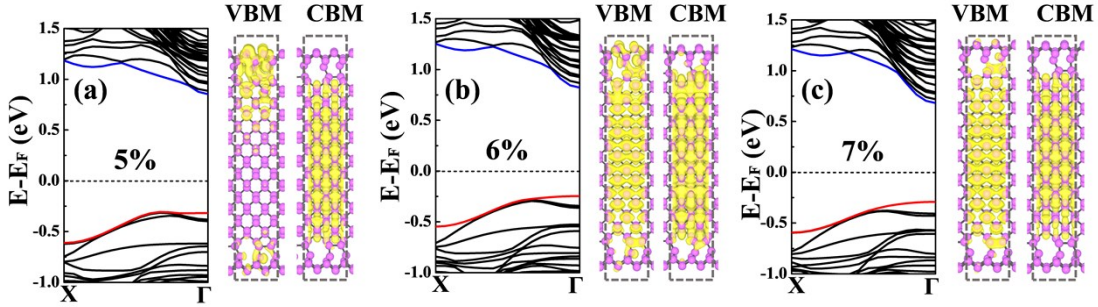

Figure S7. Electronic band structures of ZZ[Tube] PNRs with a width of 40 Å under strain of 5% ,6% and 7% (isosurface level = 1.2×10^{-5} |e|/bohr^3) (a-c). The VBM and CBM are high-lighted by red and blue, respectively.

References

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3. J. P. Perdew, K. Burke and M. Ernzerhof, *Physical Review Letters*, 1996, **77**, 3865-3868.
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