

Tunable electronic and magnetic properties of arsenene nanoribbons

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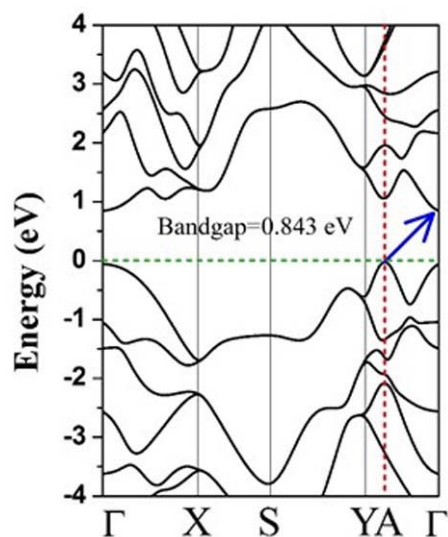


Fig. S1 Band structure of the As monolayer. The Fermi level is set to zero. The indirect band gap is indicated by the blue arrow.

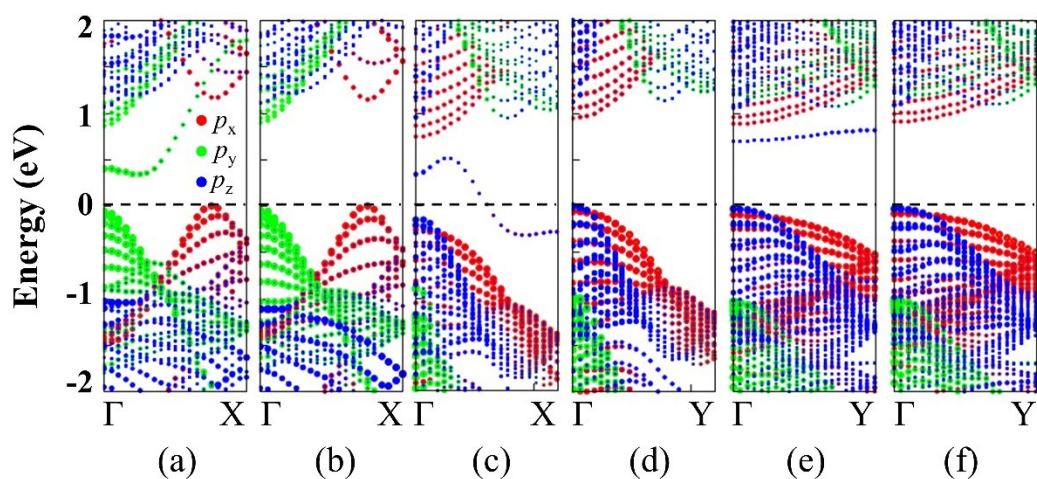


Fig. S2 Orbital-resolved band structures of the As 12-NR with the (a) unpassivated AC edge, (b) H passivated AC edge, (c) unpassivated ZZ-1 edge (nonmagnetic state), (d) H passivated ZZ-1 edge, (e) unpassivated ZZRC-o edge and (f). H passivated ZZRC-o edge. The Fermi level is set to zero.

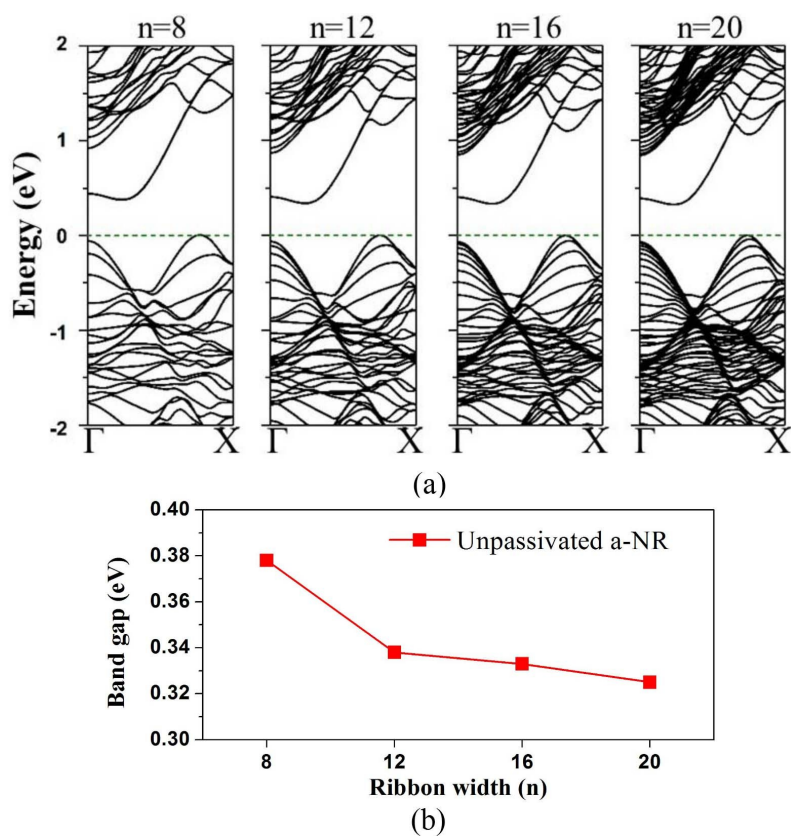


Fig. S3 (a) Band structures and (b) variation of the band gap of the unpassivated a-NRs versus ribbon width n . The Fermi level is set to zero.

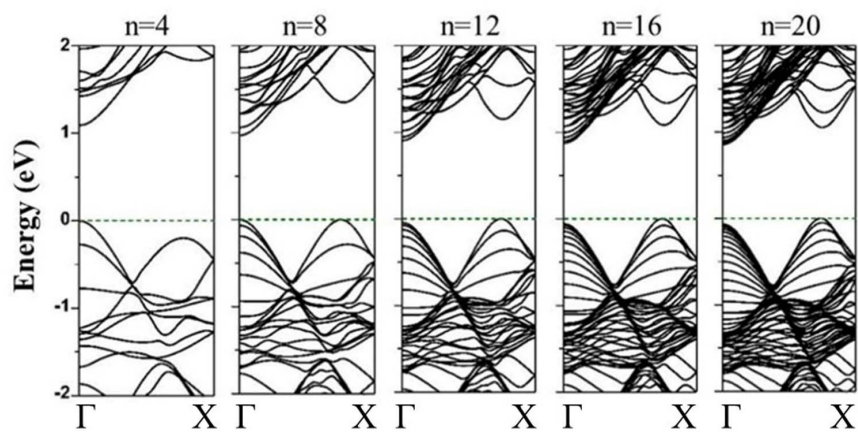


Fig. S4 Band structures of the H passivated As a-NRs versus ribbon width n . The Fermi level is set to zero.

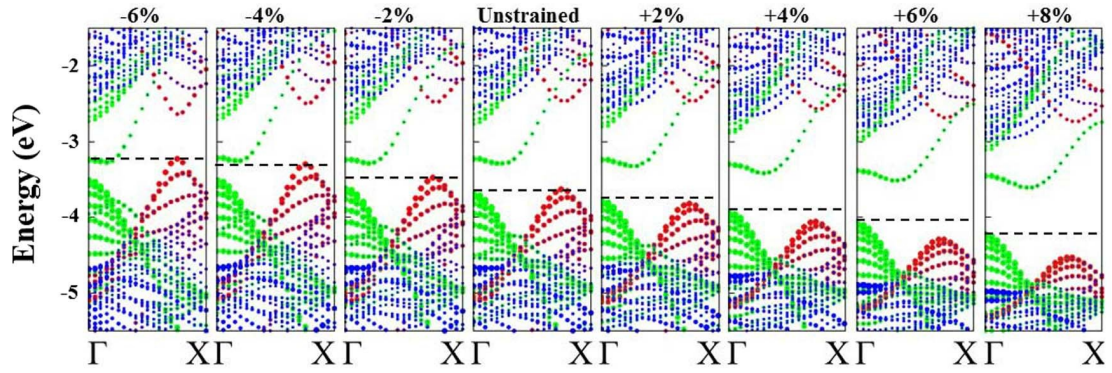


Fig. S5 Strain-dependent orbital-resolved band structures of the unpassivated As 12-a-NR. The color coding of the As p orbitals is the same as that in Fig. S2.

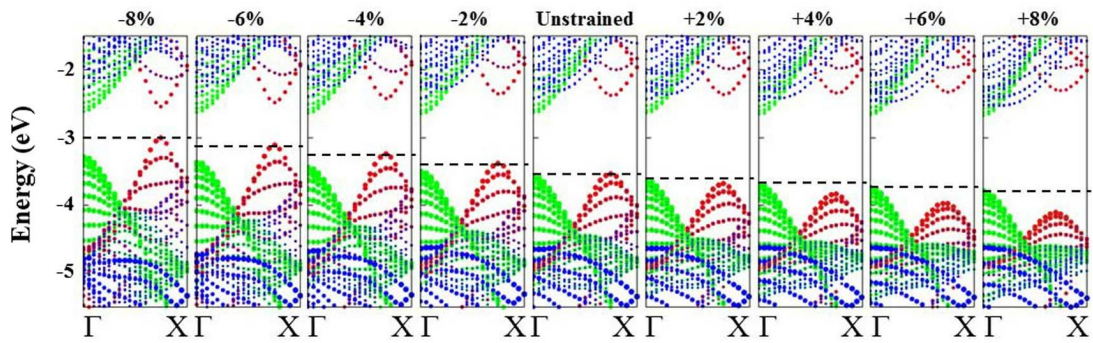


Fig. S6 Strain-dependent orbital-resolved band structures of the H passivated As 12-a-NR. The color coding of the As p orbitals is the same as that in Fig. S2.

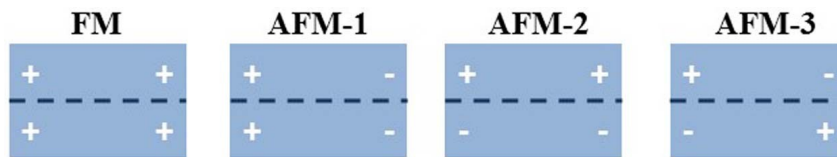


Fig. S7 Schematic view of the unpassivated As 12-z-NRs with different magnetic configurations.

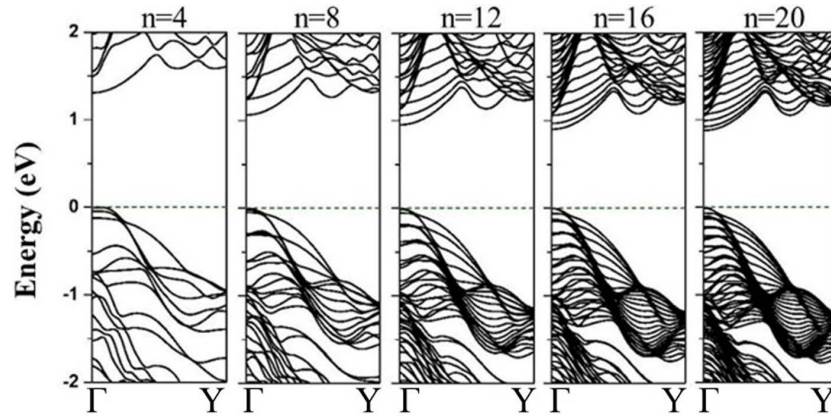


Fig. S8 Band structures of the H passivated As z-NRs versus ribbon width n . The Fermi level is set to zero.

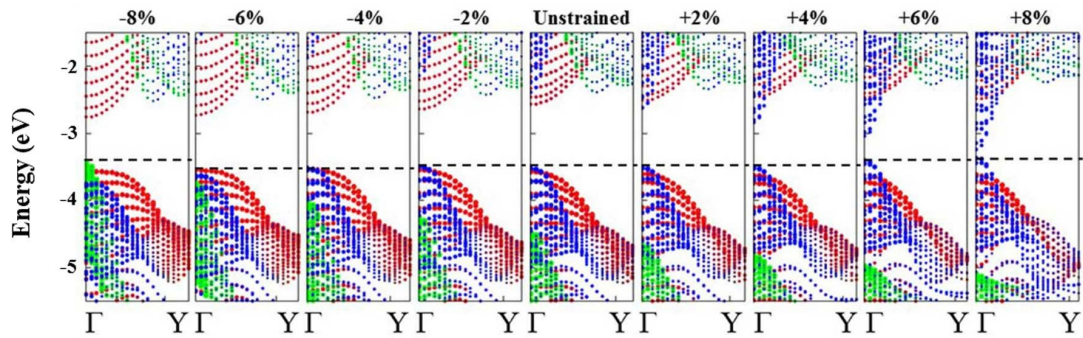


Fig. S9 Strain-dependent orbital-resolved band structures of the H passivated As 12-z-NR. The Fermi level is set to zero. The color coding of the As p orbitals is the same as that in Fig. S2.

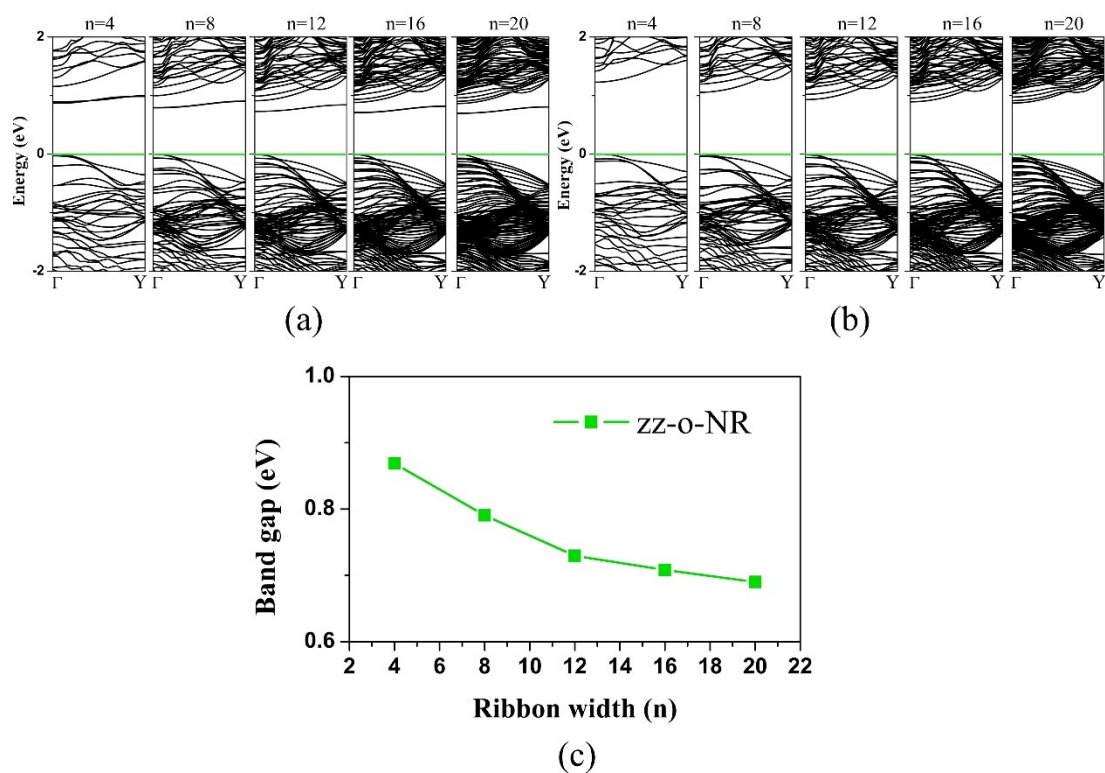


Fig. S10 (a) Band structures and (b) variation of the band gap of the zz-o-NRs versus ribbon width n . The Fermi level is set to zero.

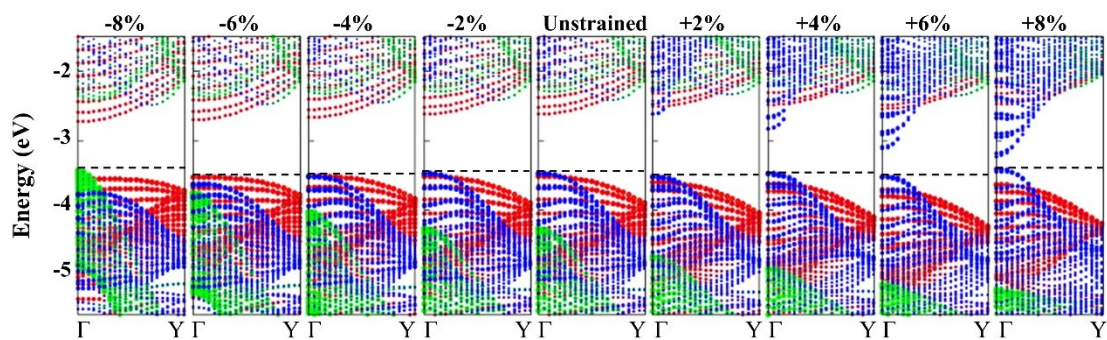


Fig. S11 Strain-dependent orbital-resolved band structures of the H passivated As 12-zz-o-NR. The Fermi level is set to zero. The color coding of the As p orbitals is the same as that in Fig. S2.

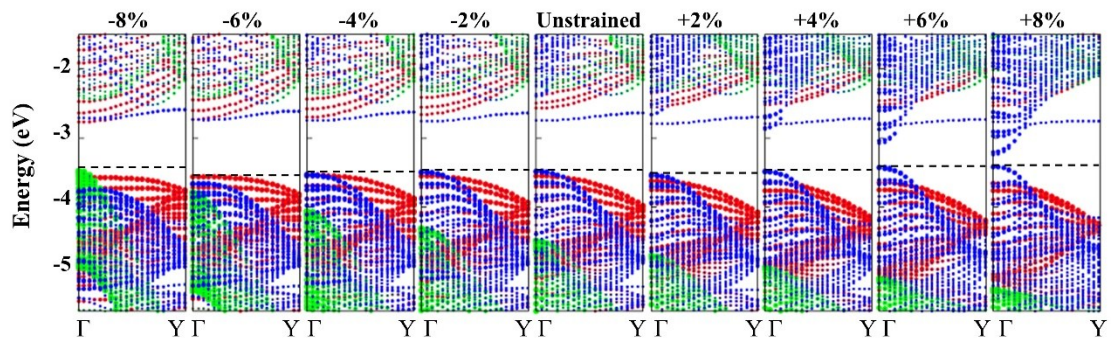


Fig. S12 Strain-dependent orbital-resolved band structures of the unpassivated As 12-zz-o-NR. The Fermi level is set to zero. The color coding of the As p orbitals is the same as that in Fig. S2.