

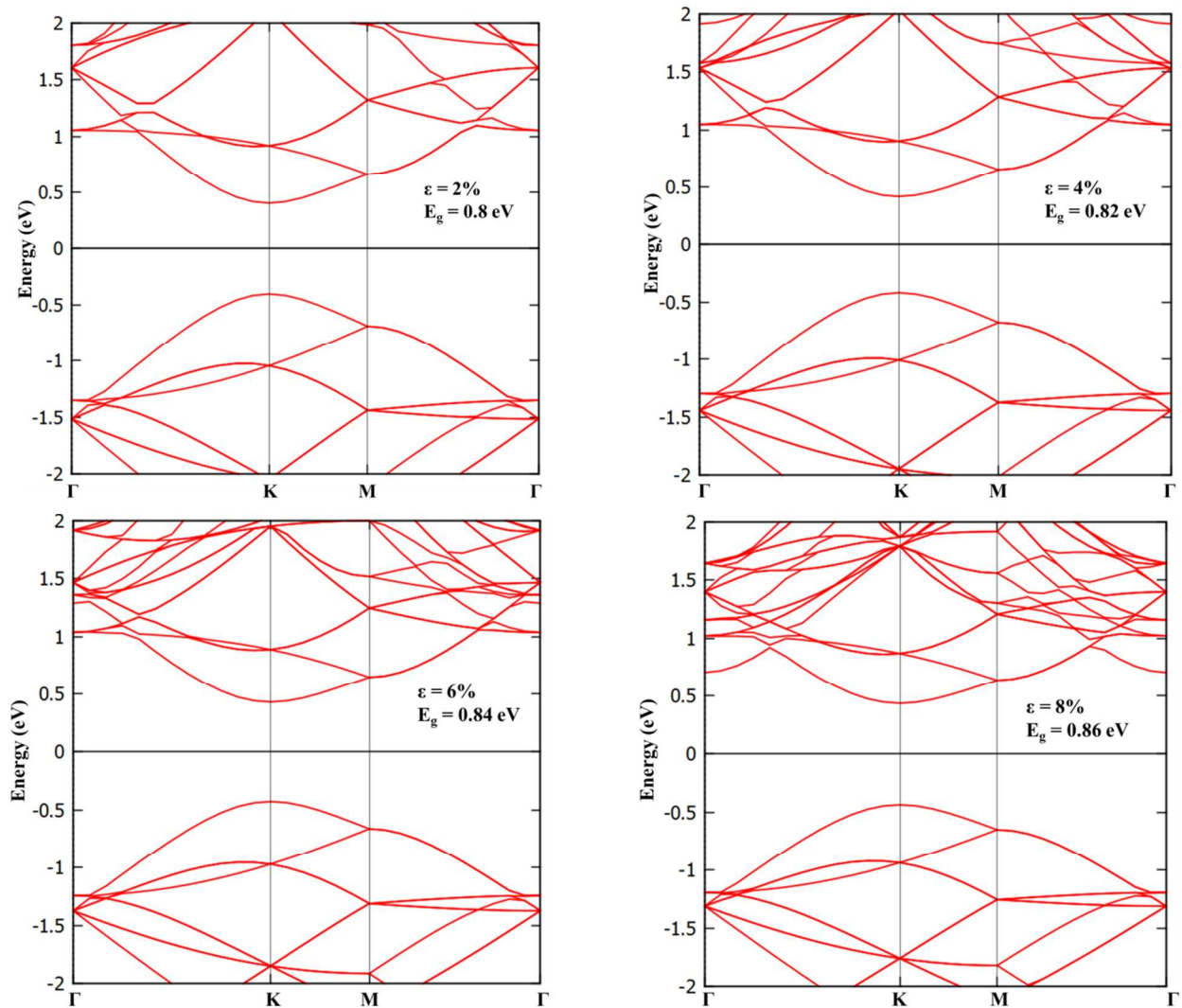
# Supporting Information

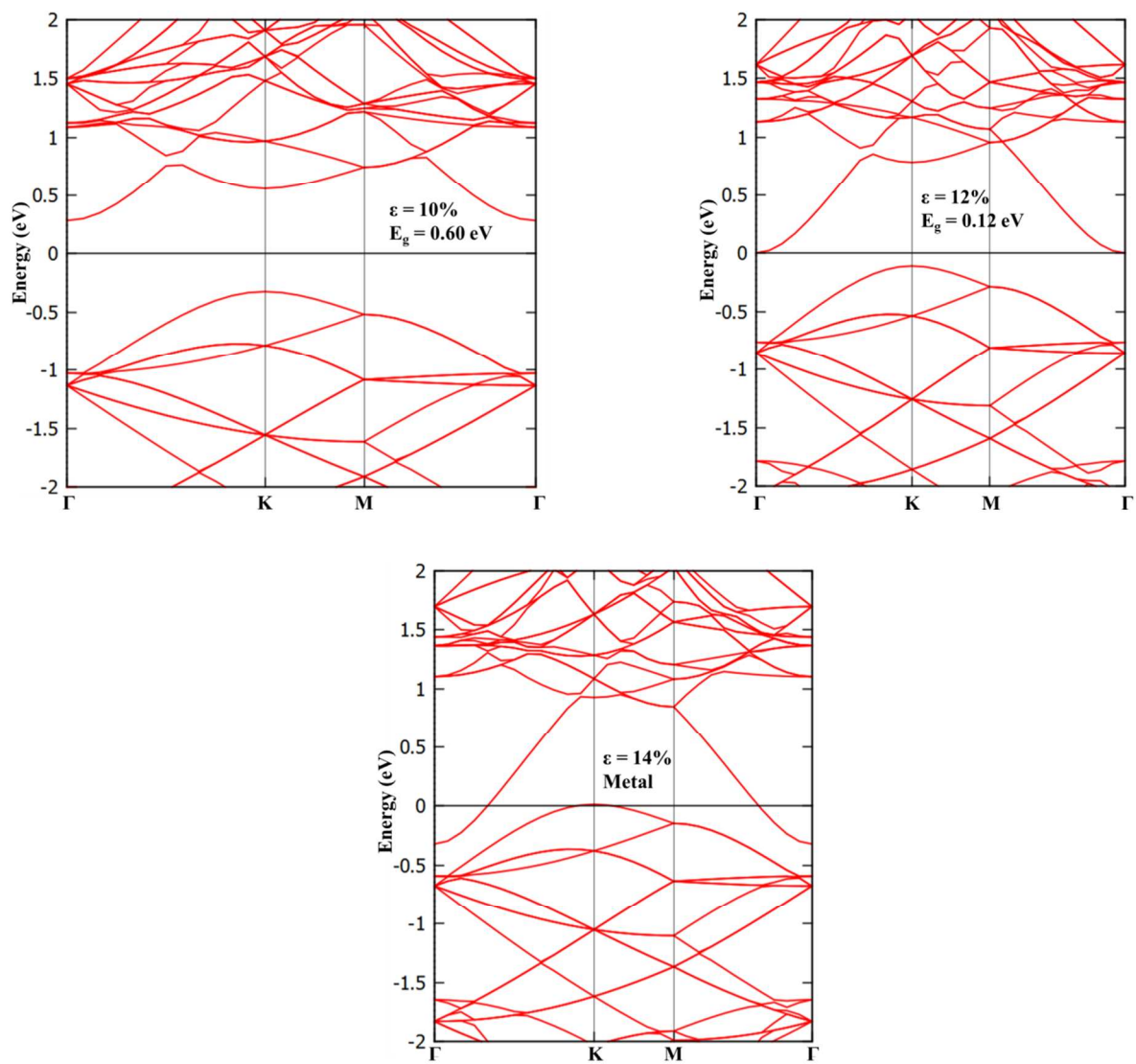
## Exploring Multifunctional Applications of Hexagonal Boron Arsenide Sheet: A DFT Study

*Kamaraj Manoharan<sup>†</sup> and Venkatesan Subramanian<sup>†\*</sup>*

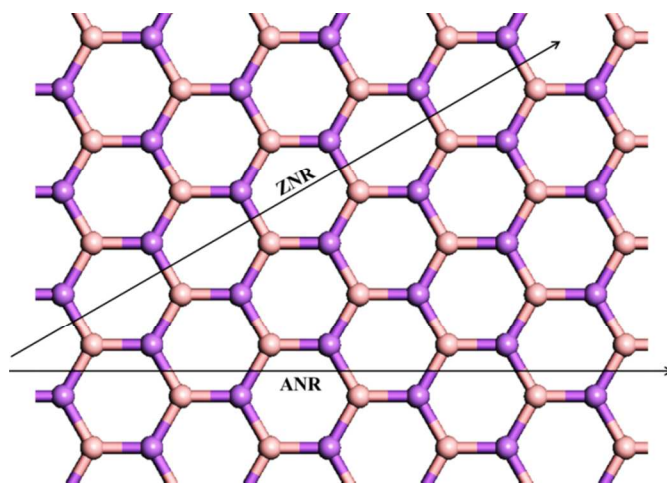
<sup>†</sup>Chemical Laboratory, Inorganic & Physical Chemistry Division, CSIR-Central Leather Research

Institute, Adyar, Chennai 600 020, India.

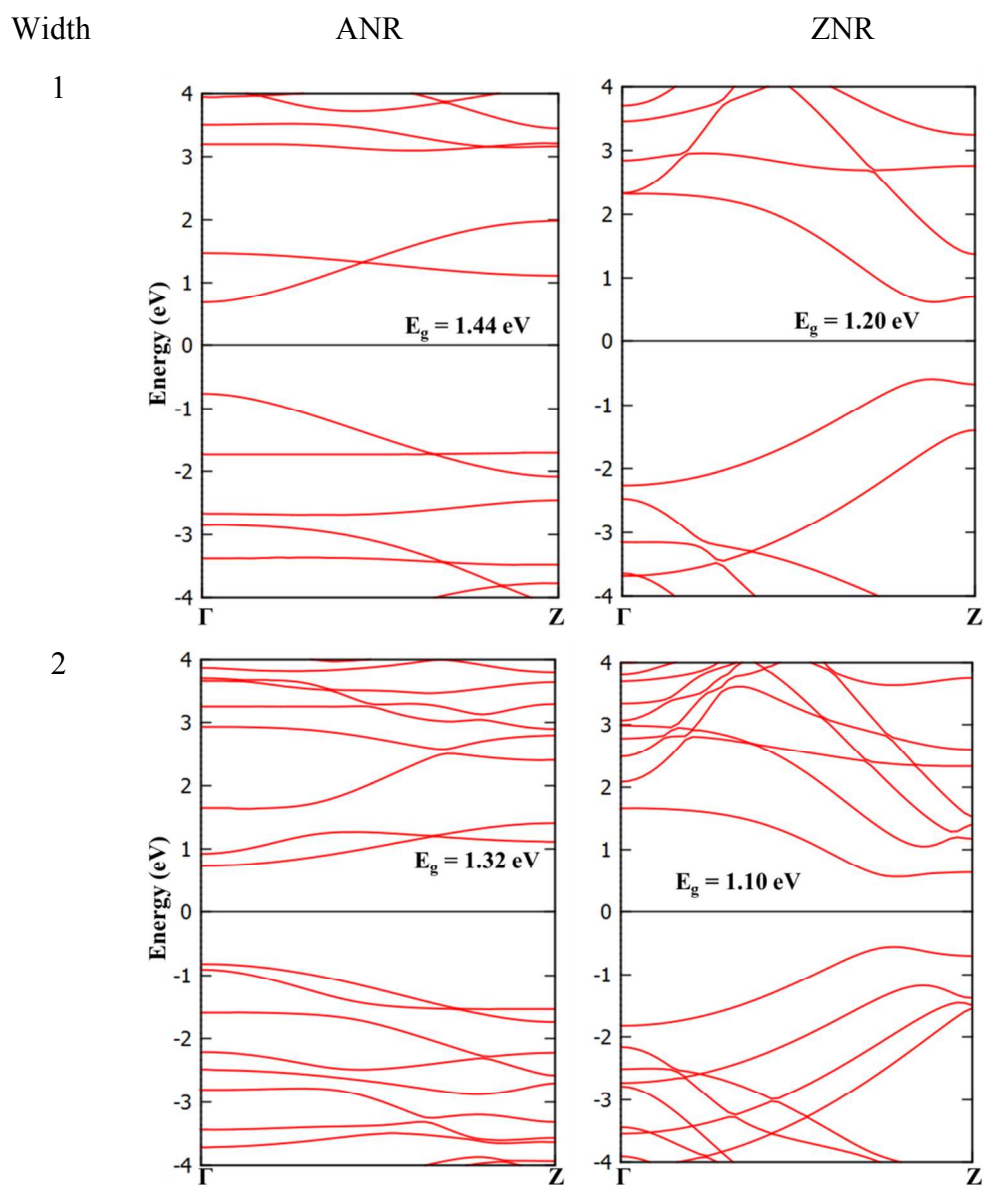




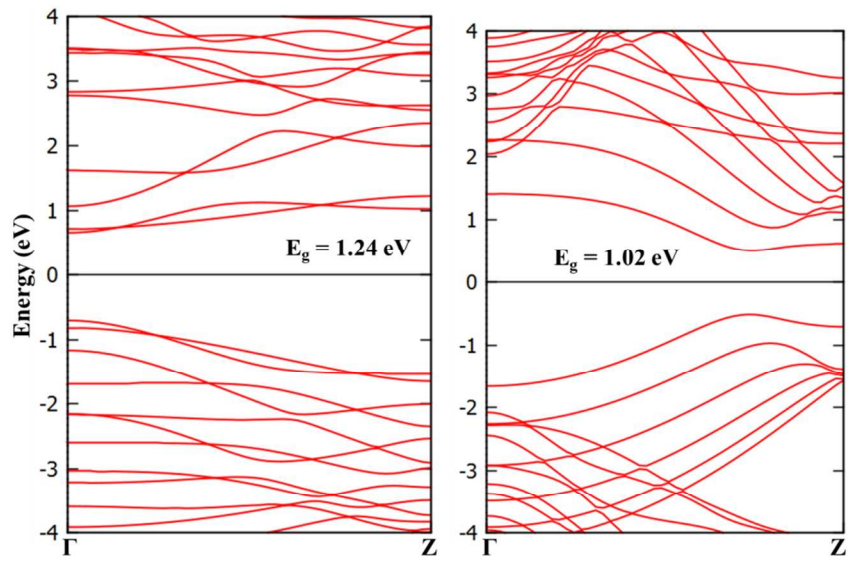
**SI Figure S1. Strain induced electronic band structure of BA sheet with different biaxial strains.**



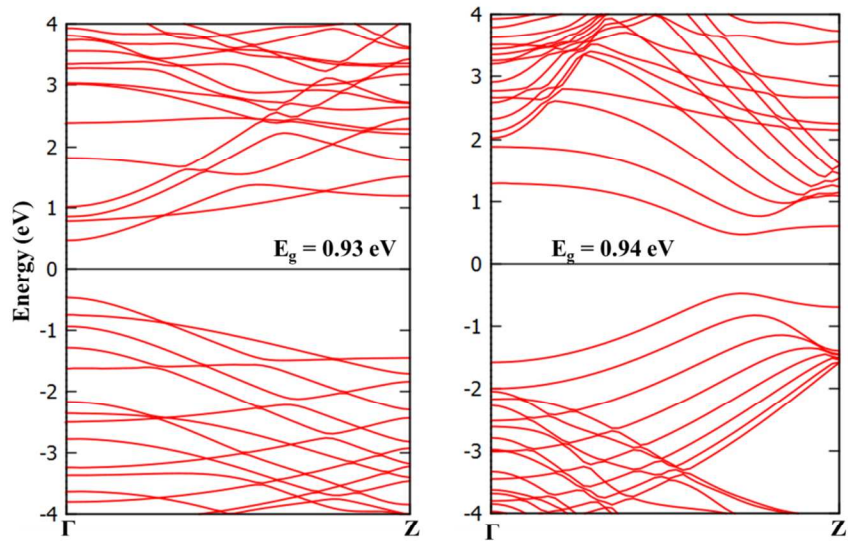
SI Figure S2. Schematic diagram of cutting 1D nano ribbons from 2D sheet



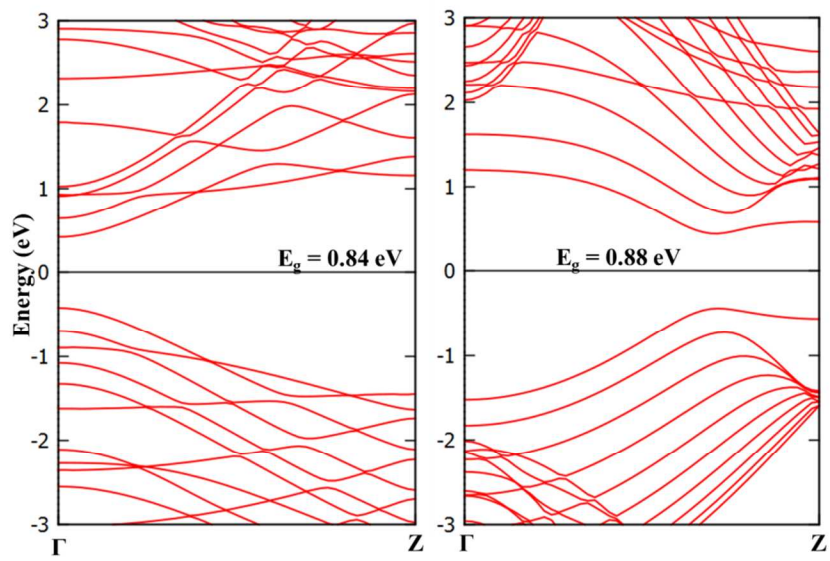
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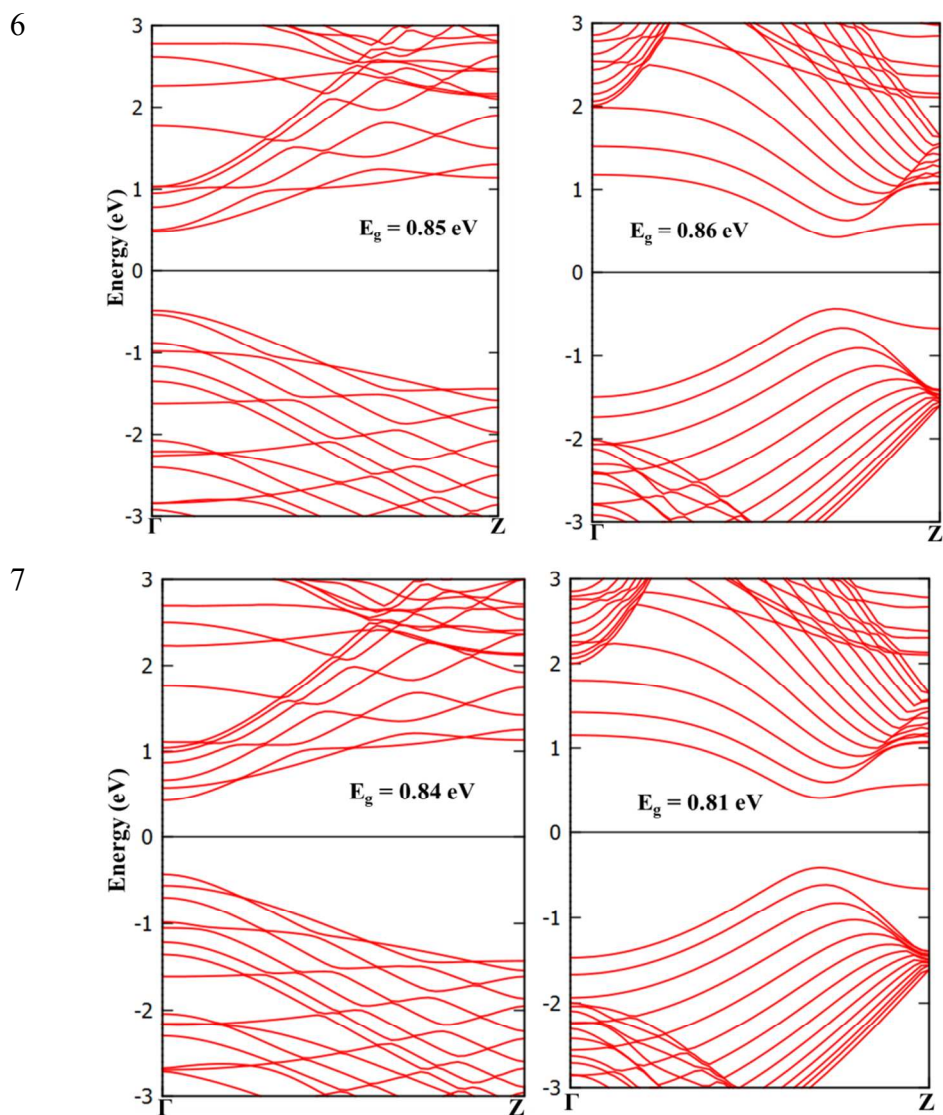
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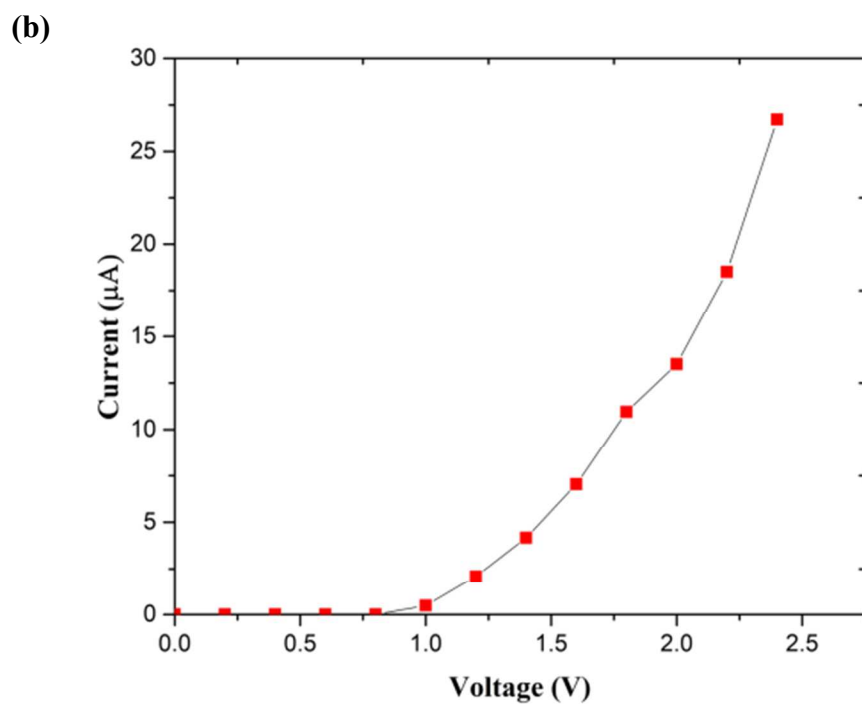
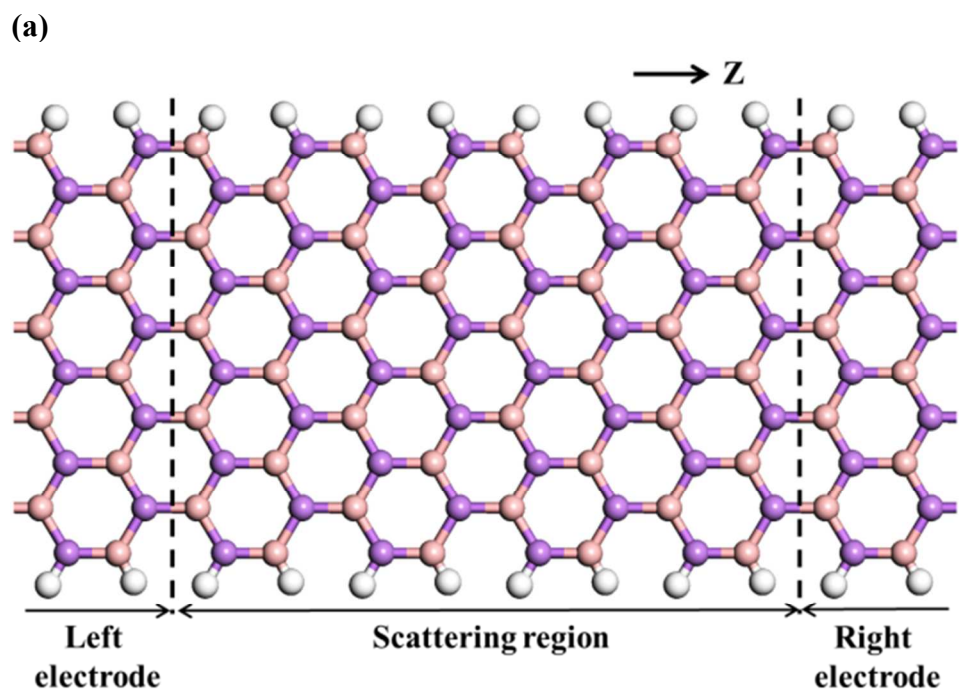




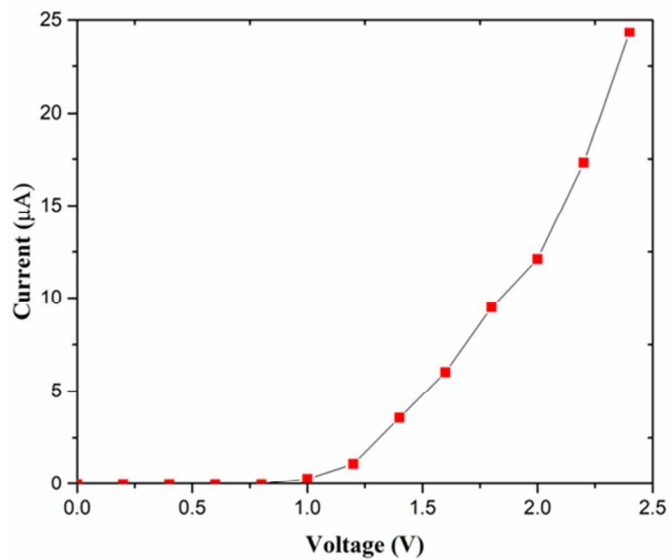
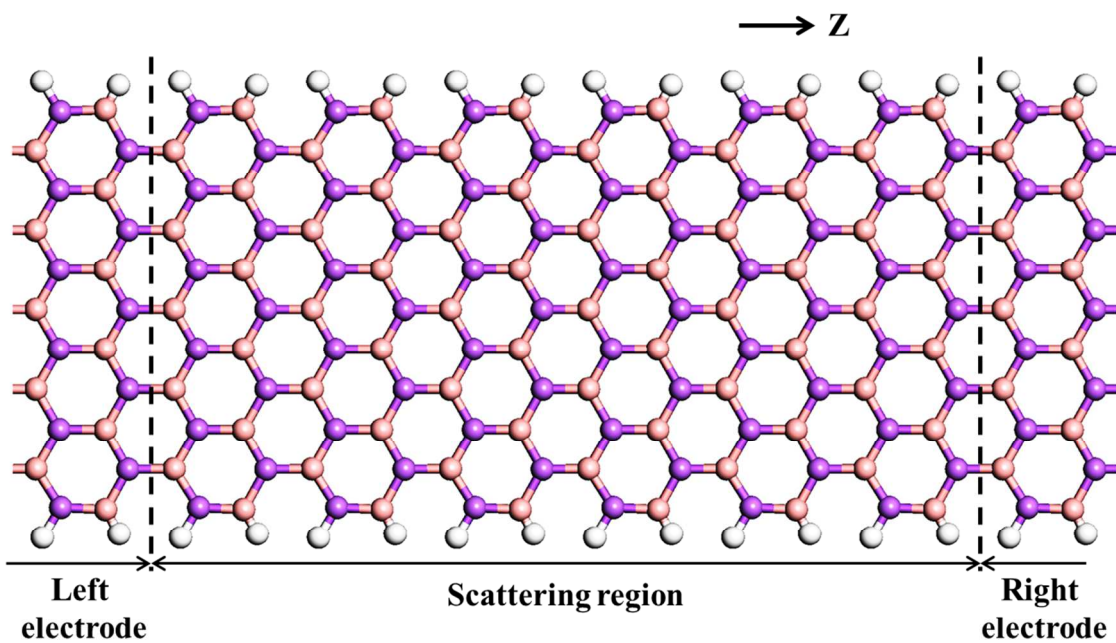
SI Figure S3. The calculated band structures of armchair and zigzag nanoribbons with various size (width  $n=1-7$ ).

SI Table T1: Wyckoff position of BAs sheet

Atom	Wyckoff position	X	Y	Z
B	1b	0.00000	0.00000	0.50000
As	1f	0.66667	0.33333	0.50000



SI Figure S4. (a) The schematic diagram of device model of 10ANR and (b) corresponding I-V characteristics



**SI Figure S5. (a) The schematic diagram of device model of 11ANR with increased scattering length and (b) corresponding I-V characteristics**