

Supplemental materials:

Strain-induced band-to-band Fermi Level Tuning in II-VI and III-V Antiphase Boundaries

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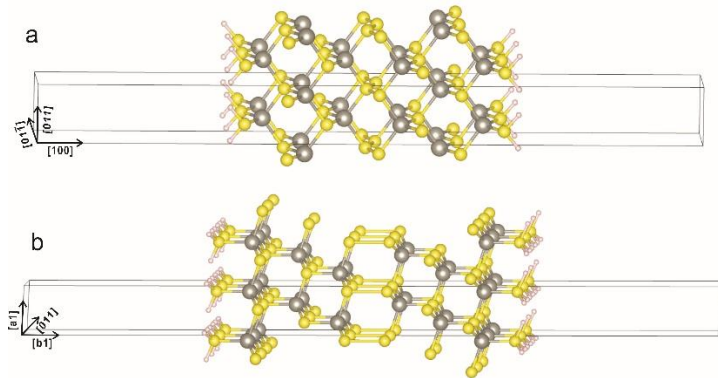


Fig.S1 The zigzag (a) and ladder (b) APB structures build for calculations.

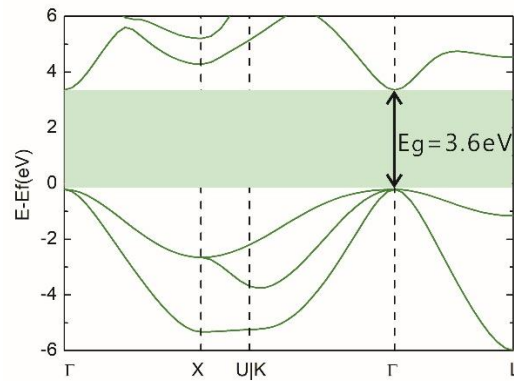


Fig.S2 Band structure of Zinc-Blende ZnS primitive cell based on HSE hybrid functional.

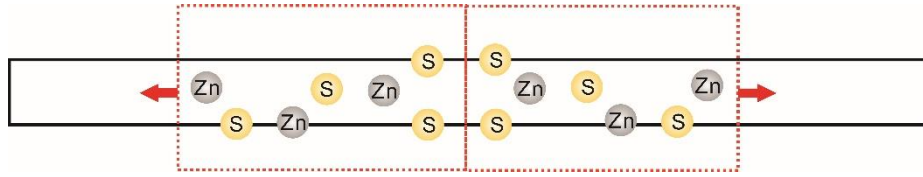


Fig.S3. Schematic diagram of the methodology used to change the APB bond lengths. The atoms are divided into two parts, and the half of atoms were translated together. In this way, the strain can be introduced only in the APB part not in the bulk atoms.

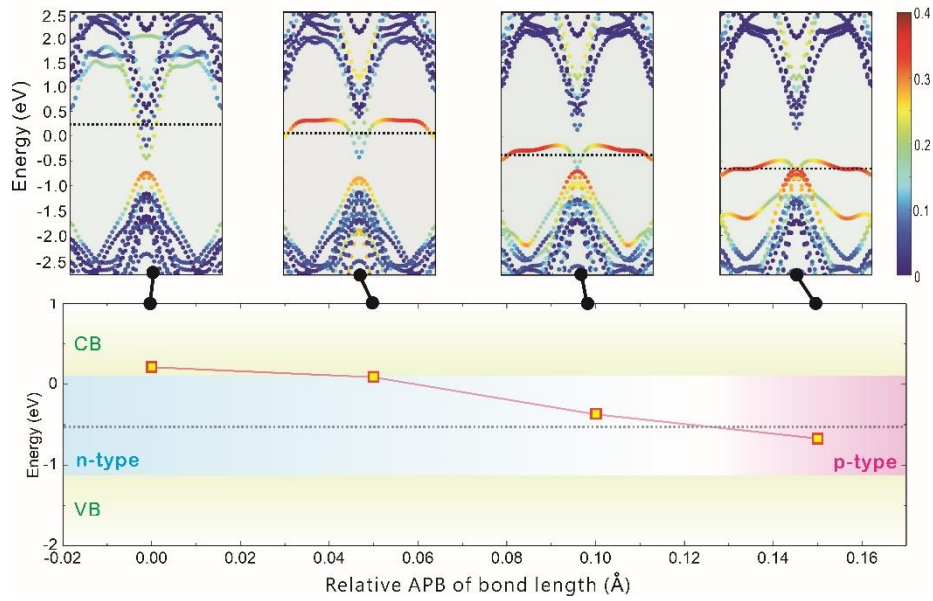


Fig.S4 APB atom-projected band structures of different ladder:P-P APB structures based on InP matrix with different APB bond lengths changed manually.