

Supporting Information

BiOCl/Group-IV Xene Bilayer Heterojunction: Stability and Electronic and Photocatalytic Properties

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In the supporting information, we first give the partial charge density of BiOCl/Xene bilayer HJs. Then, the PDOS diagrams and the band structures of BiOCl/Xene bilayer HJs under biaxial and uniaxial strain are given.

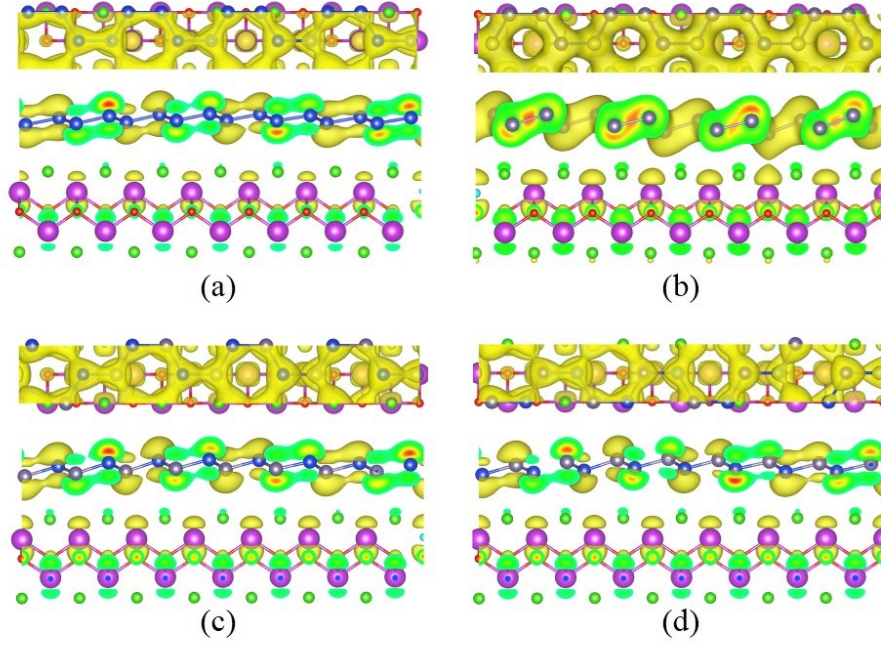


Fig. S-1 (a)-(d) The partial charge density of B/S, (b) B/G, (c) B/USG and (d) B/DSG between $\pm 0.3\text{eV}$ at Fermi level, and the isosurface value is ± 0.00032 electrons per \AA^3 .

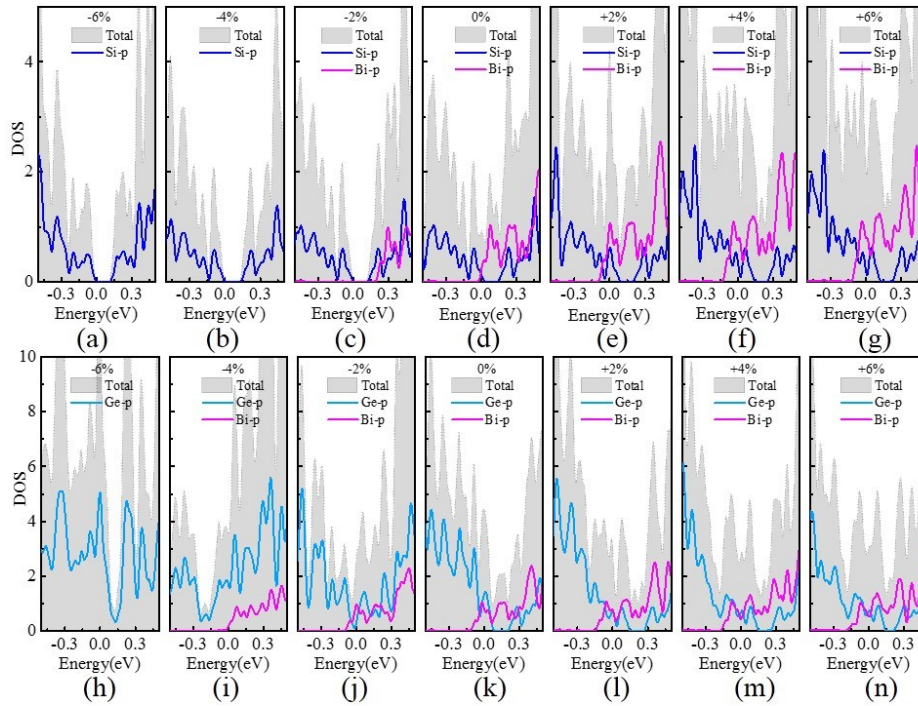


Fig. S-2 (a)-(g) PDOS diagrams of B/S under biaxial strain. (h)-(n) PDOS diagrams of B/G under biaxial strain.

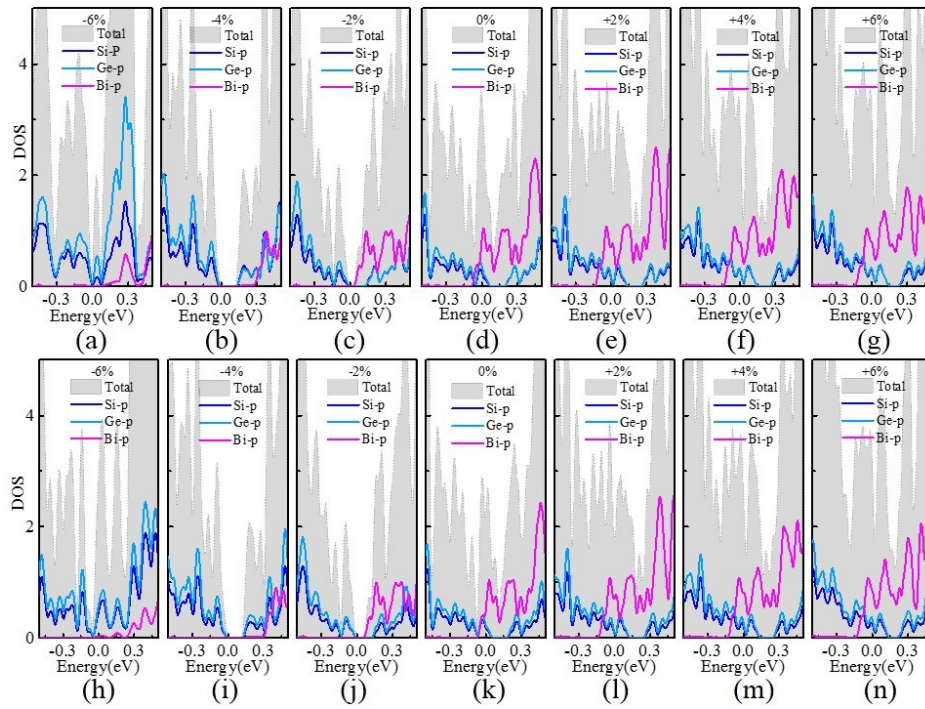


Fig. S-3 (a)-(g) PDOS diagrams of B/USG under uniaxial strain. (h)-(n) PDOS diagrams of B/DSG under uniaxial strain.

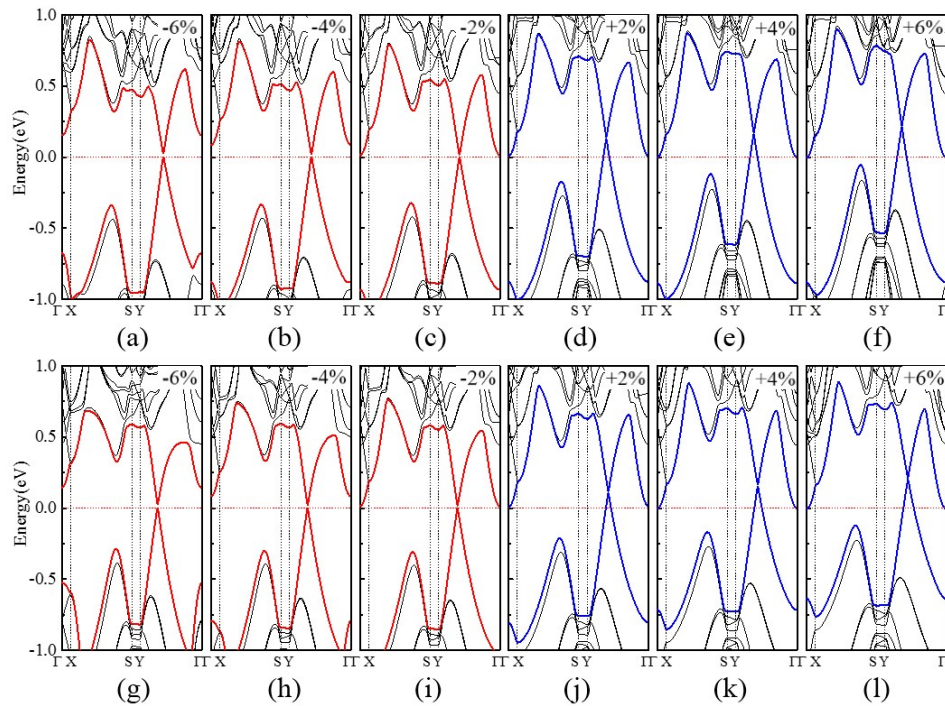


Fig. S-4 (a)-(f) Band structures of B/S under x-direction uniaxial strain. (g)-(l) Band structures of B/S under y-direction uniaxial strain.

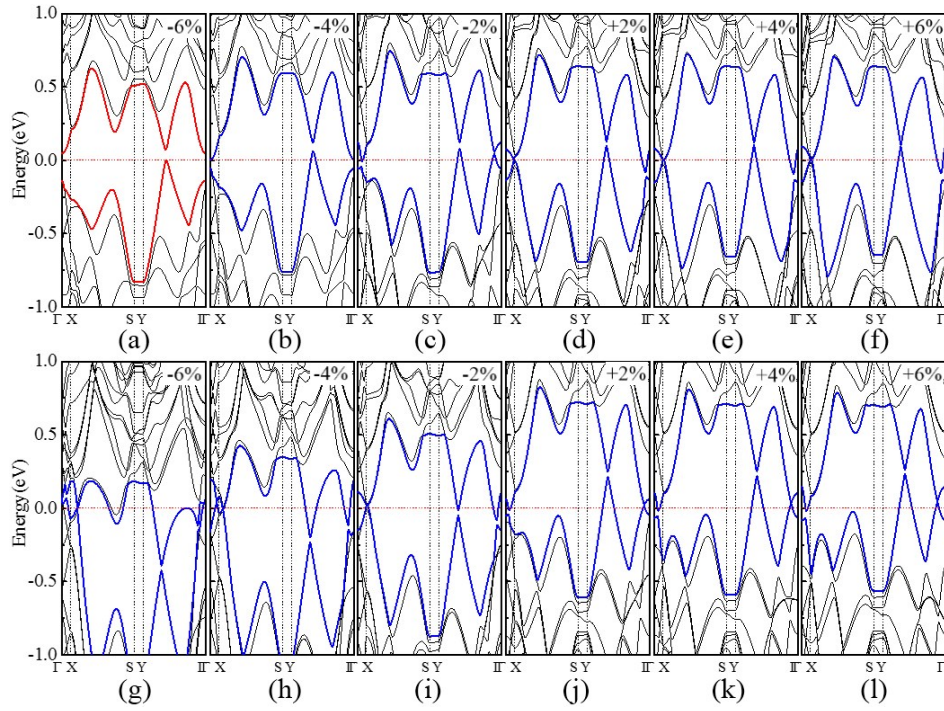


Fig. S-5 (a)-(f) Band structures of B/G under x-direction uniaxial strain. (g)-(l) Band structures of B/G under y-direction uniaxial strain.

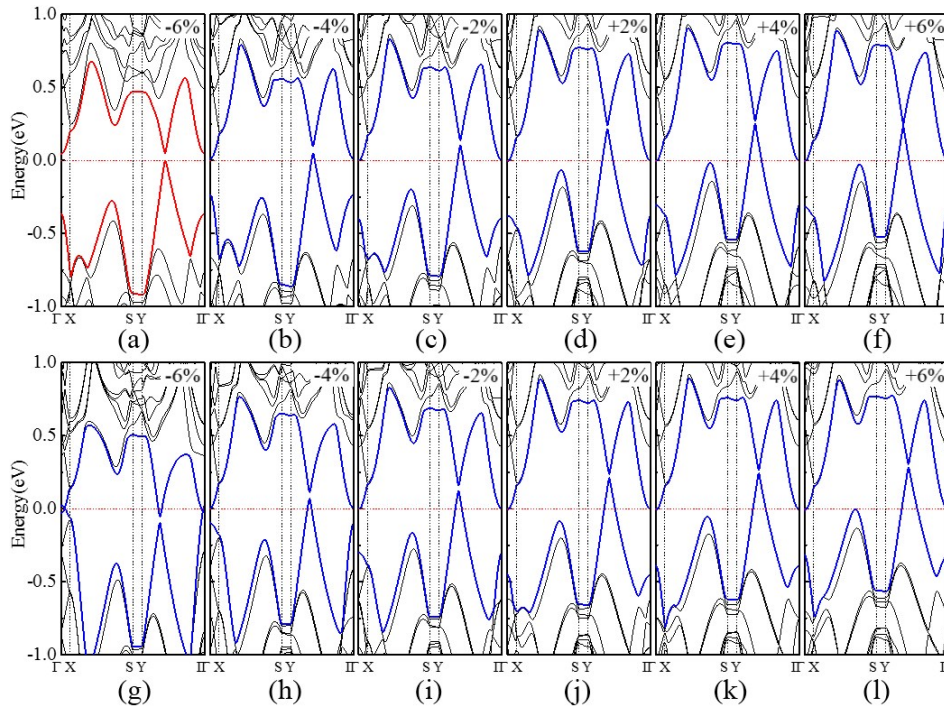


Fig. S-6 (a)-(f) Band structures of B/USG under x-direction uniaxial strain. (g)-(l) Band structures of B/USG under y-direction uniaxial strain.

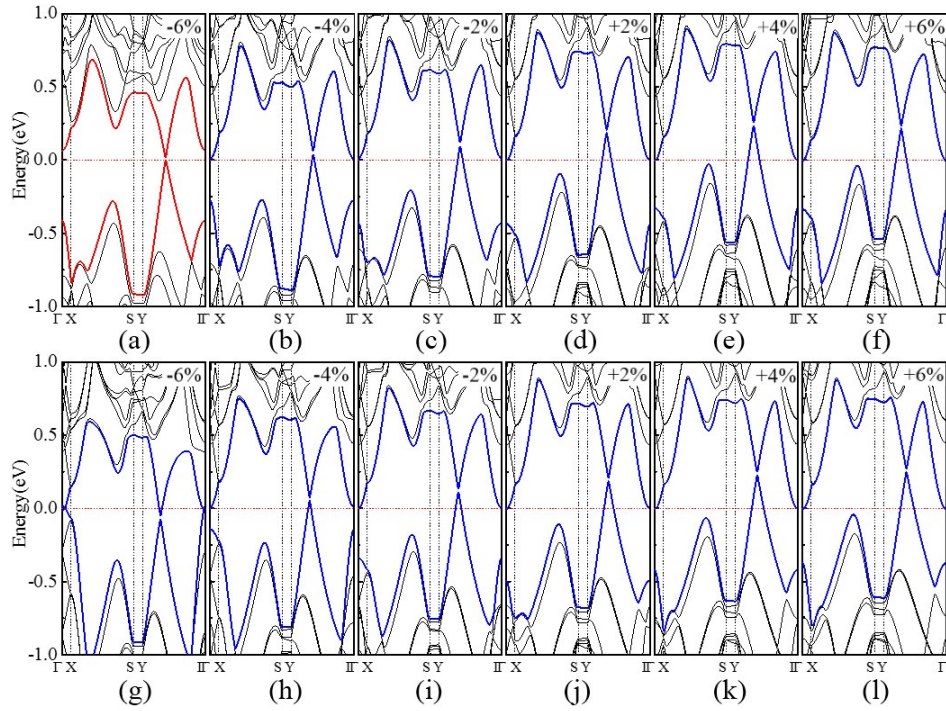


Fig. S-7 (a)-(f) Band structures of B/DSG under x-direction uniaxial strain. (g)-(l) Band structures of B/DSG under y-direction uniaxial strain.

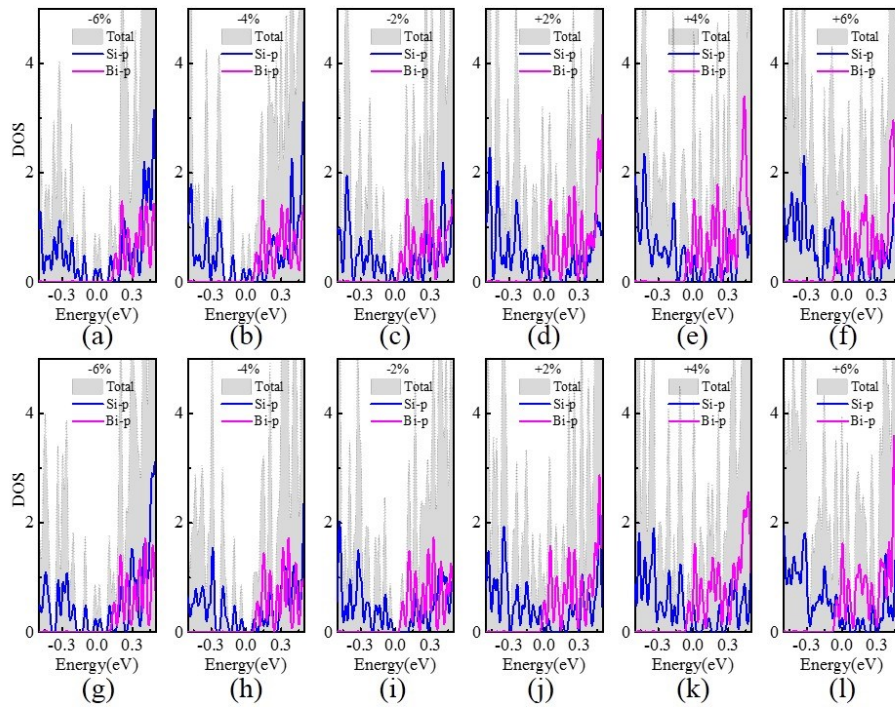


Fig. S-8 (a)-(f) PDOS diagrams of B/S under x-direction uniaxial strain. (g)-(l) PDOS diagrams of B/S under y-direction uniaxial strain.

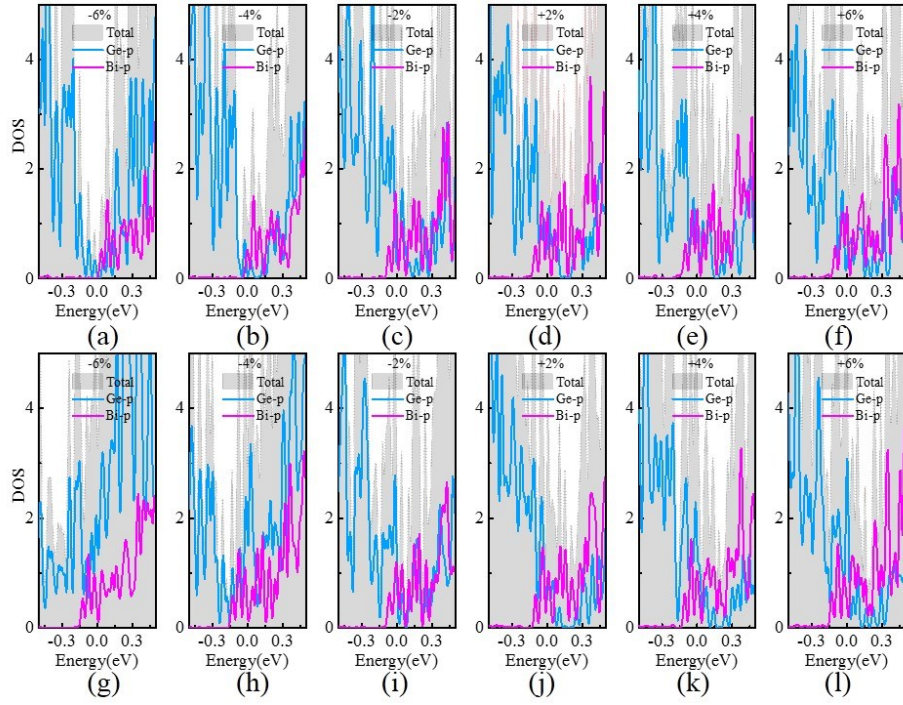


Fig. S-9 (a)-(f) PDOS diagrams of B/G under x-direction uniaxial strain. (g)-(l) PDOS diagrams of B/G under y-direction uniaxial strain.

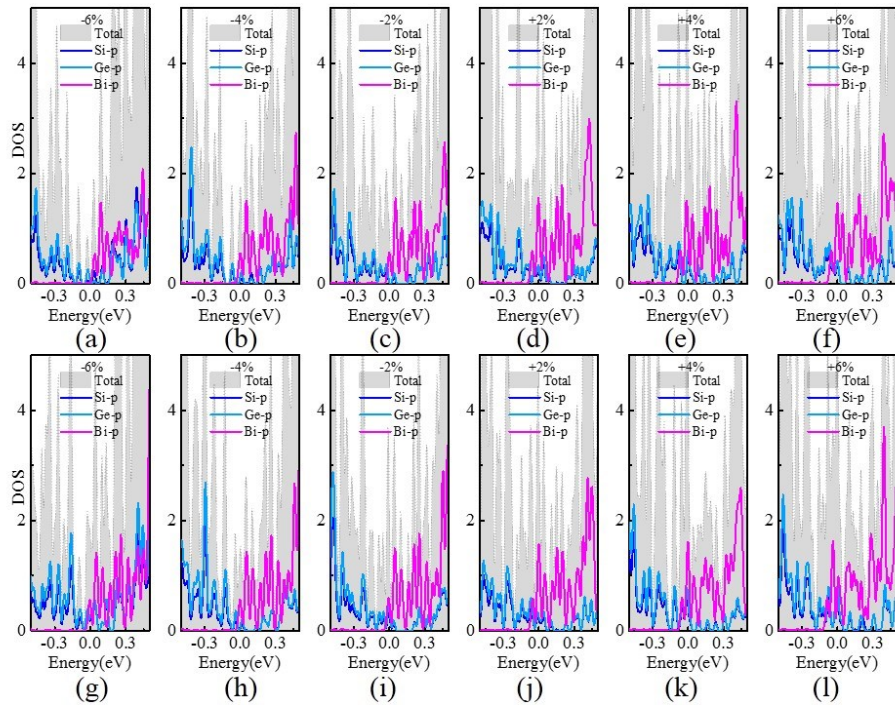


Fig. S-10 (a)-(f) PDOS diagrams of B/USG under x-direction uniaxial strain. (g)-(l) PDOS diagrams of B/USG under y-direction uniaxial strain.

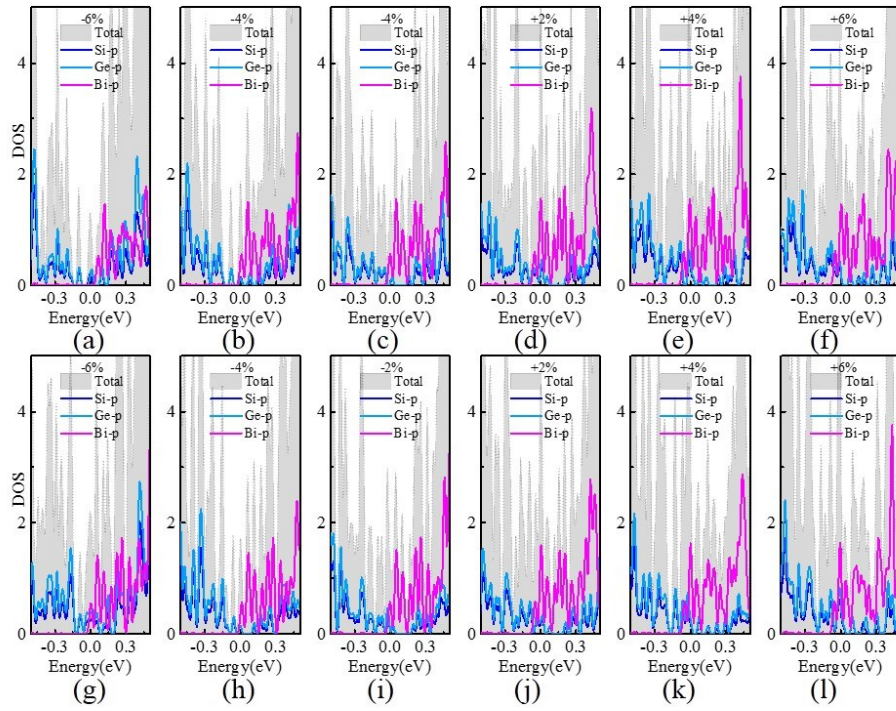


Fig. S-11 (a)-(f) PDOS diagrams of B/DSG under x-direction uniaxial strain. (g)-(l)

PDOS diagrams of B/DSG under y-direction uniaxial strain.