Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary Information

Structural phase transition of BiSb and formation of Weyl semimetallic phase under pressure: calculations and experiments

Bulk bandstructure is calculated with and without-SOC. Fig. S1(a-h) represent the calculated electronic bandstructure along the high symmetry lines of the hexagonal Brillouin zone. BiSb is an indirect semiconductor at atmospheric pressure in both with and without-SOC. The band gap is 0.119 eV with-SOC and less than 0.198 eV without-SOC. Moreover, due to the presence of SOC, each band of BiSb shows spin-splitting. At 4 GPa, the conduction band broadening is more obvious and the semi-metallic behavior is remarkable.

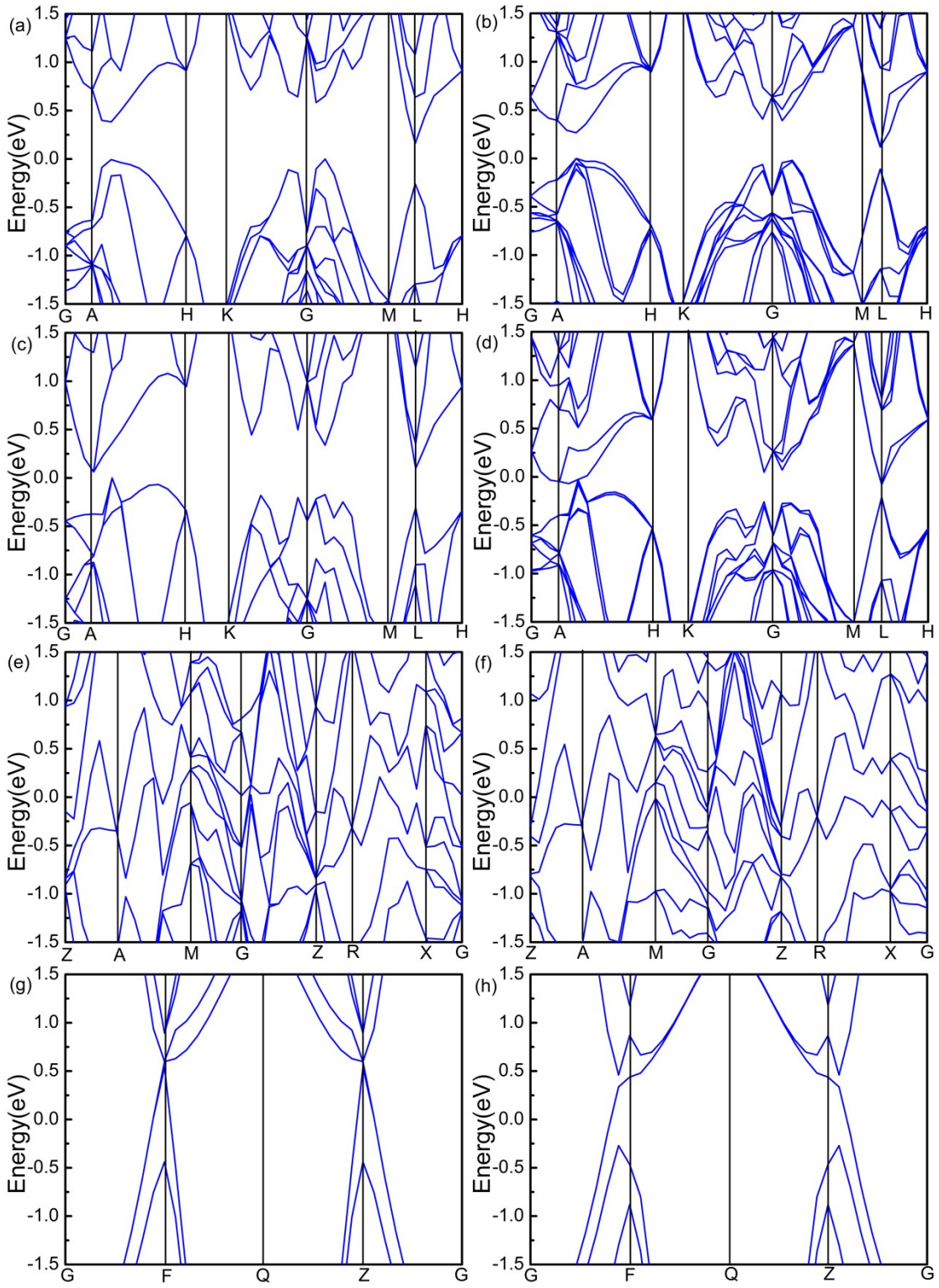

Fig. S1 Bandstructures (a,c,e and g) without-SOC and (b,d,f and h) with SOC are at 0 GPa, 4 GPa, 15 GPa and 25 GPa, respectively.

In order to further explore the bonding and estimate the amount of electrons on and between the participating atoms, we have performed Mulliken-population analysis. The calculated Mulliken charges are listed in Table S1 for all BiSb.

TABLE S1. Mulliken-population analysis for the BiSb at different pressures. The Mulliken charges are given in terms of *e*.

BiSb	Atom	Mulliken charges
0 GPa	Sb	0.83
	Bi	-0.84
4 GPa	Sb	-1.4
	Bi	1.4
15 GPa	Sb	1.27
	Bi	-1.27
25 GPa	Sb	0.95
	Bi	-0.97

The ability of Sb atoms to obtain electrons at 4 GPa is enhanced, indicating that the interlayer Bi-Sb interaction is enhanced, as observed in ELF.