Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information for

Two-dimensional Semimetal AlSb monolayer with multiply nodal-loops and extraordinary transport property under uniaxial strains

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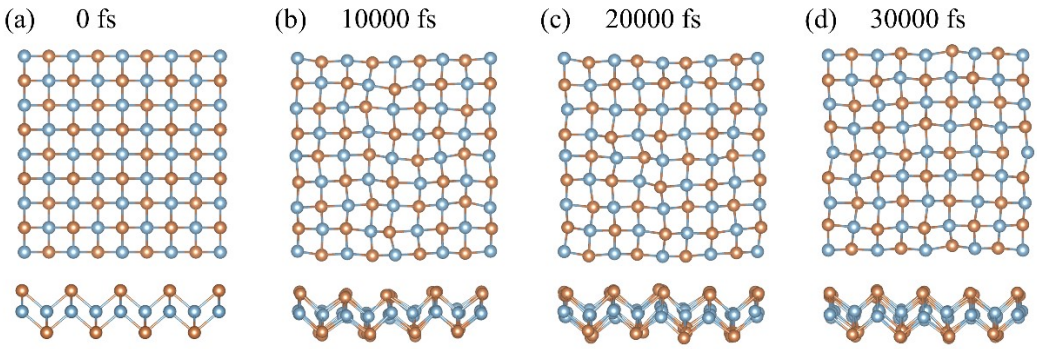
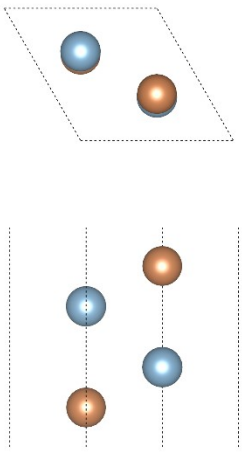
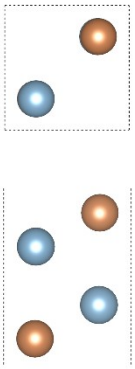
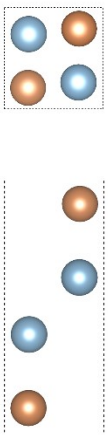


Fig. S1 (a-d) Snapshots of geometric structure for AlSb monolayer during AIMD simulation at 0ps, 10ps, 20ps and 30ps, respectively.

Table S1 Configurations of OsN2 from global searches based on CALYPSO package.

Configuration	Relative Energy (eV)	Space Group
	0.000eV/atom	C2/M

	0.028eV/atom	P4/NNM
	0.087eV/atom	ABM2
	0.122eV/atom	P4/NMM
	0.161eV/atom	P21/M

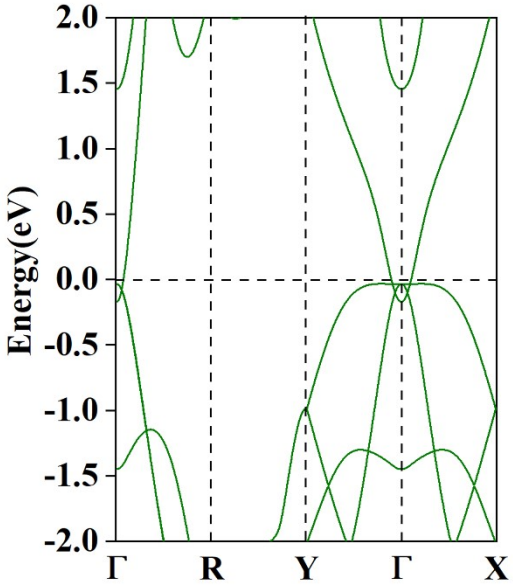


Fig. S2 Band structure of AlSb monolayer calculated with HSE06 functions.

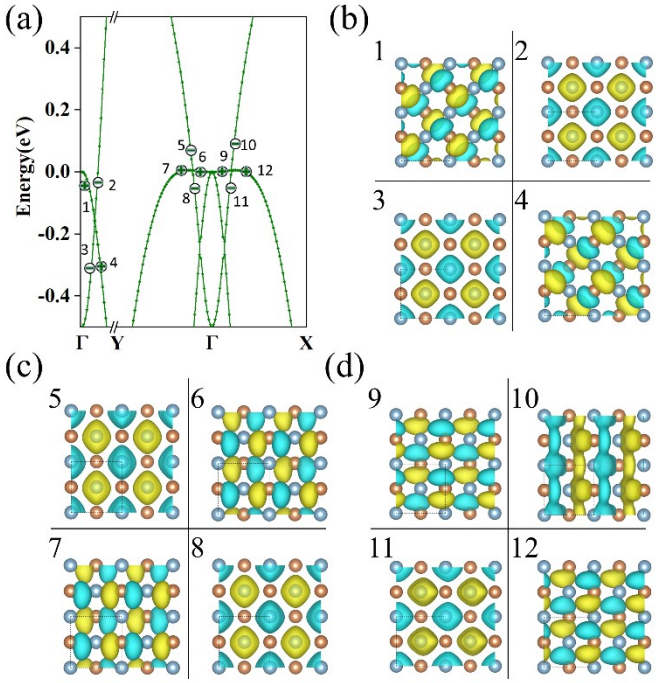


Fig. S3 (a) Calculated band structure of AlSb monolayer. (b-d) Real part of Kohn-Sham wave functions near band crossing points.

Symmetry protection mechanism on NLs

When we move one Al atom by 0.05 Å along the x-direction, as shown in Fig. S4 (a), the loop degenerates into four line segments. When we move one Al atom by 0.05 Å in the x direction and the other by 0.05 Å in the y direction, as shown in Fig. S4 (b), the upper and lower energy bands are completely separated. In this scenario, the NL nature is destroyed due to the band gap opening (274.8meV, 46.8meV, and 559.0meV) at three band crossing. To be brief, the glide mirror plays an indispensable role for protecting the NL state in AlSb monolayer.

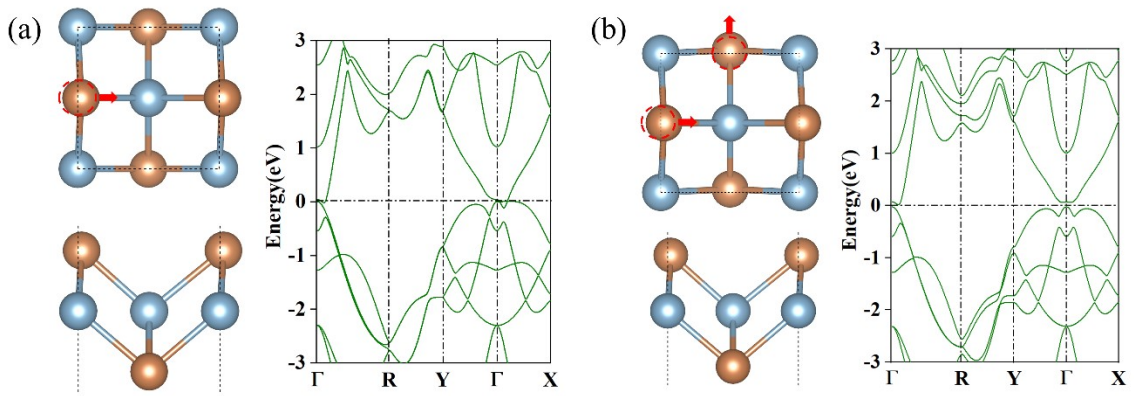


Fig. S4 Top and side views of geometric structure and the band structure for distorted AlSb monolayer. The red dotted line represents the equilibrium position of Al atom. (a) One Al atom moves 0.05 Å in the x direction and another Al atom is in the equilibrium position. (b) One Al atom moves 0.05 Å in the X direction and another Al atom moves 0.05 Å in the Y direction.

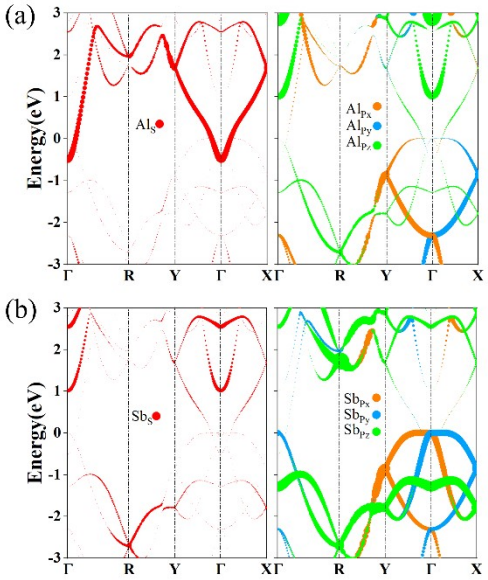


Fig. S5 corresponding orbital-resolved projection from (a) Al atom and (b) Sb atom.

The family of Hamiltonians is

$$H(k) = \varepsilon_s \times U_1 + \varepsilon_p \times U_2 + t_1 \times U_3 + t_2 \times U_4 + t_s \times U_5 + t_p \times U_6,$$

in which

$$U_1 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$U_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$U_3 = \begin{bmatrix} 0 & h_{12} & 0 & 0 & 0 & 0 \\ h_{21} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$h_{21} = h_{12} = \left(e^{iak_x} + e^{iak_y} + e^{ia(k_x + k_y)} + 1\right) \times e^{-\frac{ia(k_x + k_y)}{2}}$$

$$U_4 = \begin{bmatrix} h_{11} & 0 & 0 & 0 & 0 & 0 \\ 0 & h_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$h_{11} = h_{22} = 2\cos ak_x + 2\cos ak_y$$

$$U_5 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & h_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & h_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & h_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & h_{66} \end{bmatrix}$$

$$h_{33} = h_{55} = 2\cos ak_x,\ h_{44} = h_{66} = 2\cos ak_y$$

$$U_6 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & h_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & h_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & h_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & h_{66} \end{bmatrix}$$

$$h_{33} = h_{55} = 2\cos ak_y,\ h_{44} = h_{66} = 2\cos ak_x$$

Table S2 Slater-Koster tight-binding parameters of AlSb with a lattice constant a = b = 4.22 Å and interlayer distance d = 20 Å in the absence of SOC. Unit: eV.

ε_s	ε_p	t_1	t_2	t_s	t_p
7.9	-2.5	-1.3	-0.8	1.2	0.05

Effects of Symmetry Breaking

$$U_7 = \begin{bmatrix} 0 & 0 & 0 & -2i\sin\frac{ak_y}{2} & 0 & 0 \\ 0 & 0 & 2i\sin\frac{ak_x}{2} & 0 & 0 & 0 \\ 0 & -2i\sin\frac{ak_x}{2} & 0 & 0 & 0 & 0 \\ 2i\sin\frac{ak_y}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$U_8 = \begin{bmatrix} 0 & 0 & 0 & 0 & 2i\sin\frac{ak_x}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & -2i\sin\frac{ak_y}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -2i\sin\frac{ak_x}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 2i\sin\frac{ak_y}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

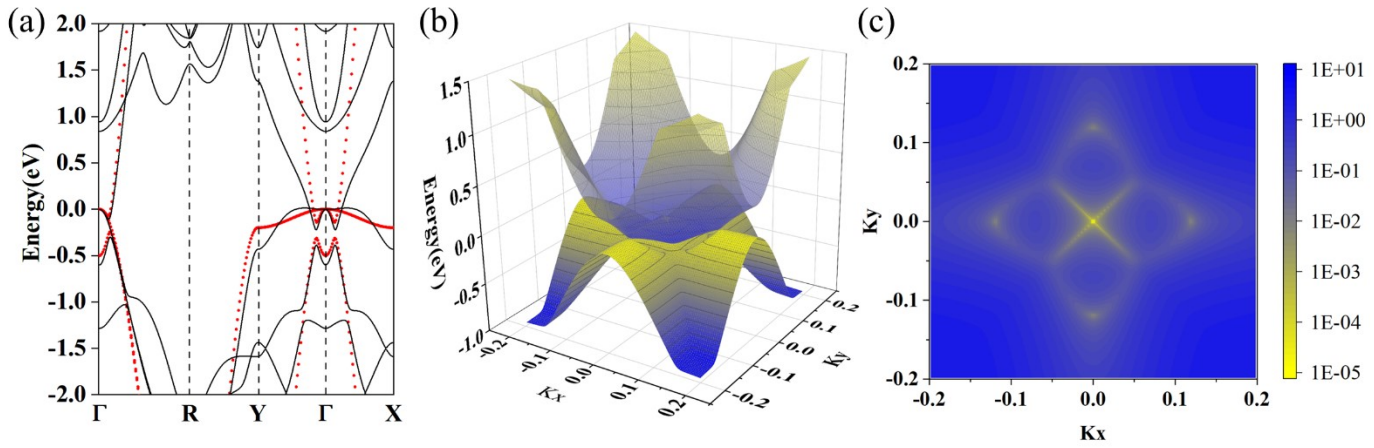


Fig. S6 (a) Electronic band structures under electric field from first-principles calculations (black solid line) and tight-binding model (red dotted line). (b) 3D energy band structure with the effect of electric field. (c) In-plane projection of the electronic band structure.

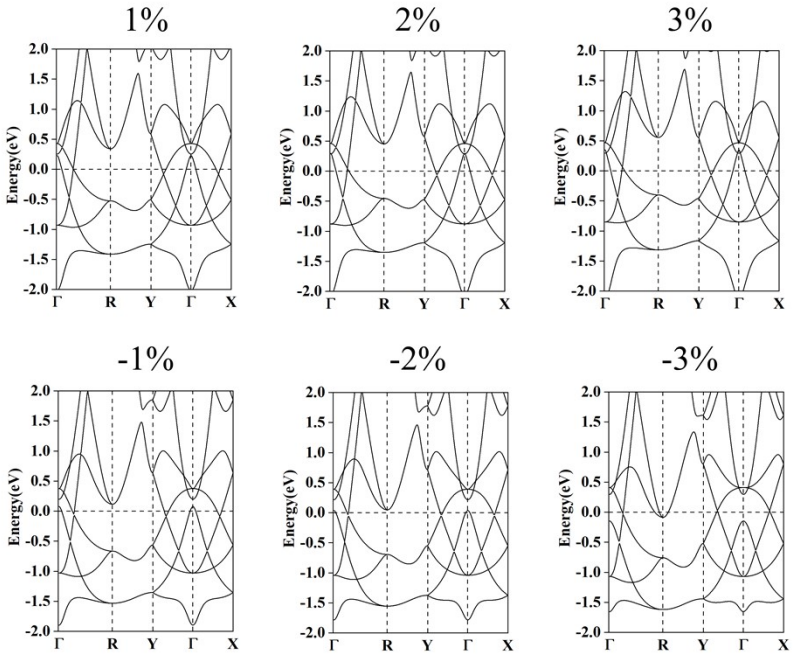


Fig. S7 Band structure obtained for oxidized AlSb monolayer under biaxial in-plane strains.

Discussions on the thermoelectric properties of AlSb monolayer

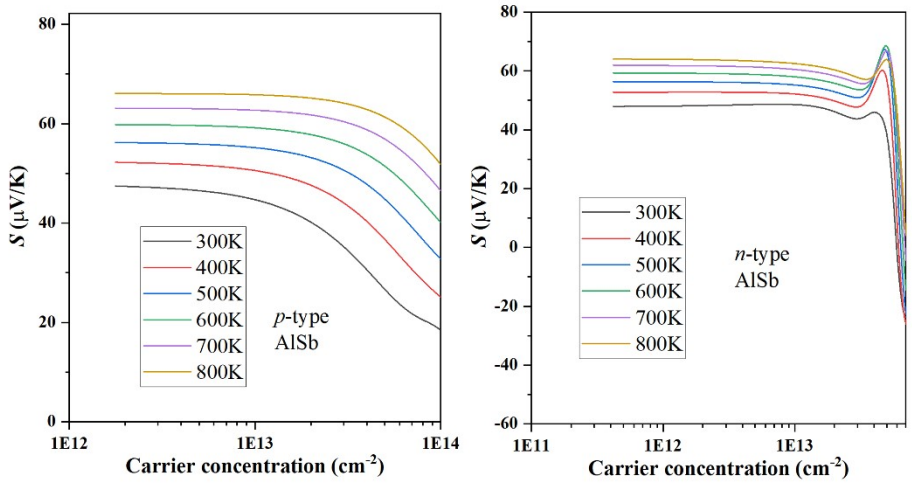


Figure. S8 The calculated Seebeck coefficients *S* of the *p*-type and *n*-type AlSb as a function of carrier concentration at the temperature of 300–800 K.

We studied the Seebeck coefficient of AlSb monolayer using the Vienna ab initio simulation package combined with the BoltzTrap2 package. In order to obtain more accurate results, the energy cutoff was fixed at 600 eV, and the Brillouin zone was sampled by a 51 × 51 × 1 Γ-centered Monkhorst-Pack k-point mesh. Based on the obtained band structure, the transport properties are obtained the semi-classical Boltzmann theory based on the relaxation time approximation. The Seebeck coefficient *S* of the *p*-type and *n*-type AlSb as a function of carrier concentration at the temperature of 300-800 K are shown in Figure S8. The *S* is large at high carrier concentrations and shows a similar variation tendency for all the considered temperature. For the *n*-type carrier, the maximum absolute value of *S* for AlSb is larger than that for *p*-type AlSb. Unfortunately, the Seebeck coefficient of AlSb (~60$\mu V/K$) is orders of magnitude lower than that of other typic 2D thermoelectric materials such as black phosphorus (~2000 $\mu V/K$) and GeS (~2800 $\mu V/K$), indicating that AlSb monolayer is scarcely possible to have good thermoelectric performance.