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Supporting information

Direct band gap and anisotropic transport of ZnSb monolayers tuned by hydrogenation and strain

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To check the mechanical stability of hydrogenated ZnSb monolayers, we carry out the calculations of elastic stiffness constants of ZnSb monolayers with full hydrogenation. With the Born-Huang stability criteria as described by

$$C_{11} > 0,\ C_{22} > 0,\ C_{11} > |C_{12}|,\ C_{66} > 0,$$

the fully hydrogenated 2D ZnSb monolayers under strains of 0% and 8% are found to be mechanically stable as shown in table S1.

Table S1. Elastic Stiffness Constants of fully hydrogenated 2D ZnSb monolayer.

Strain	C_{11}(N/m)	C_{12}(N/m)	C_{22}(N/m)	C_{66}(N/m)
0%	44.000	7.119	31.255	14.554
8%	21.539	4.381	31.027	11.408

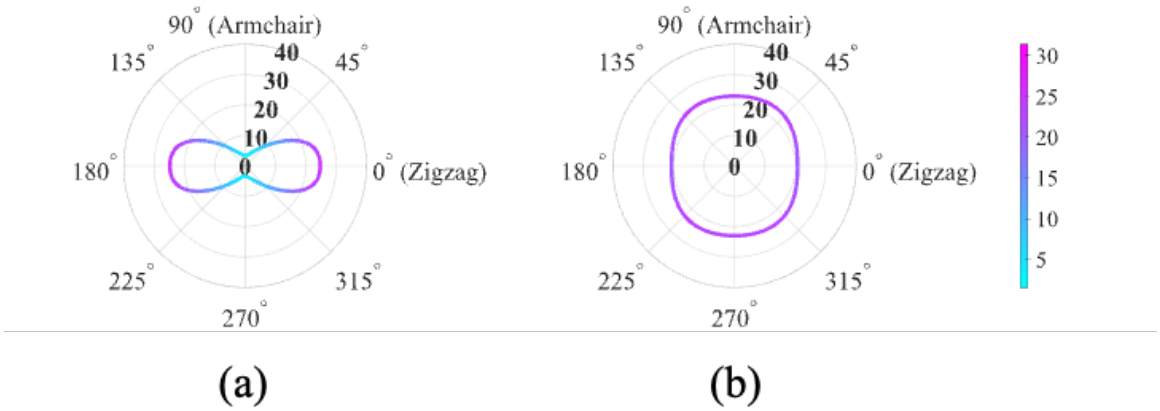

Figure S1. Young's Modulus of ZnSb monolayer sheet as a function of the in-plane angle θ with θ corresponding to the a axis (zigzag) under (a) 3% and (b) 5.5% strain.

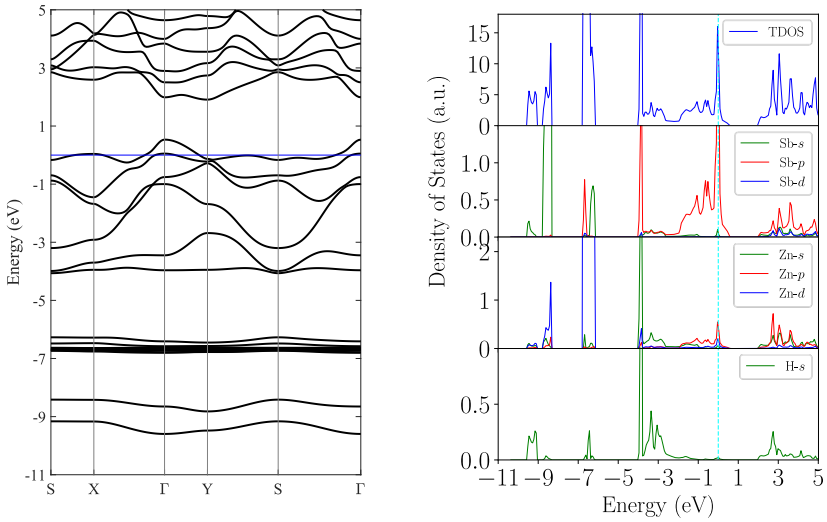

Figure S2. (a) Electronic band structure (PBE) and (b) total and orbital-projected density of states for the half hydrogenated ZnSb monolayer sheet. The Fermi level is set to zero.

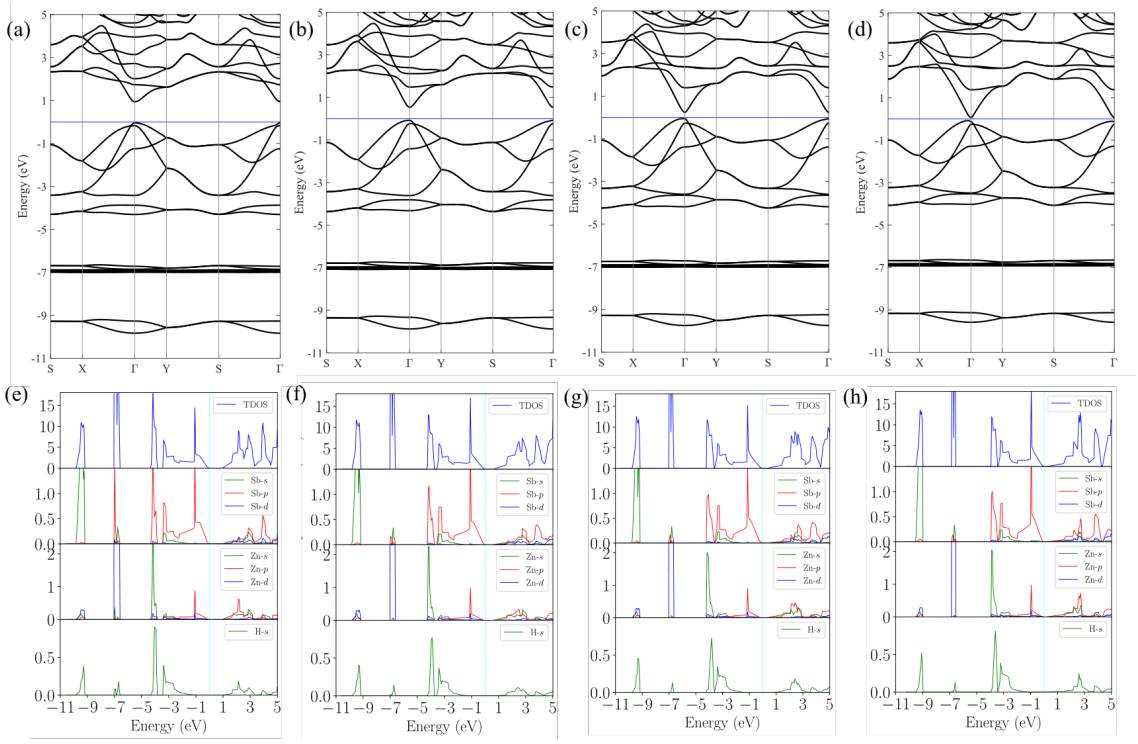

Figure S3. (a)-(d) Calculated electronic band structures (PBE) and (e)-(h) total and orbital-projected density of states for the fully hydrogenated ZnSb monolayer under strains of 2%, 4%, 6%, and 8%, respectively.

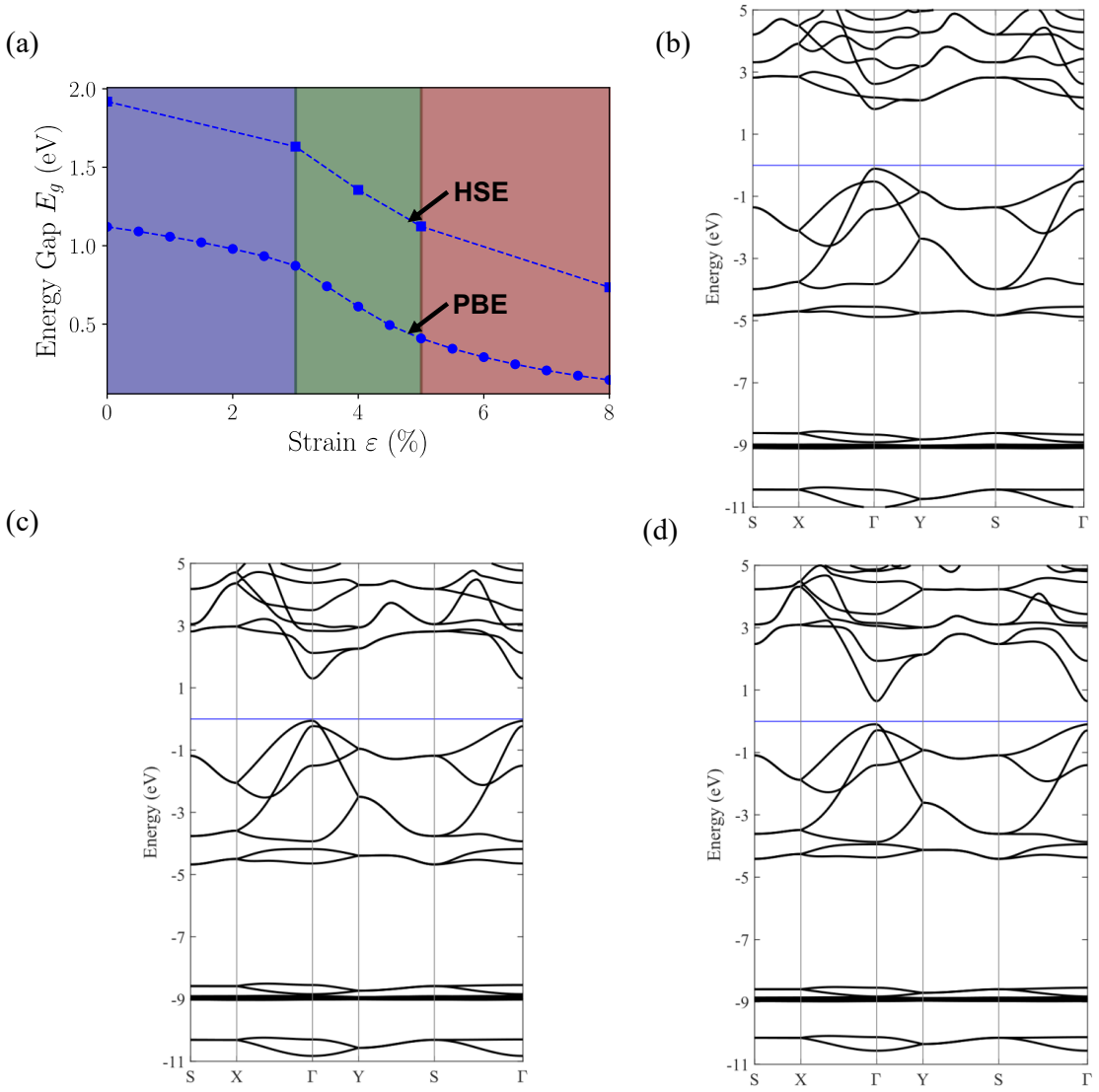

Figure S4. (a) The energy gaps E_g as a function of biaxial strain using PBE and HSE functionals. (b)-(d) Calculated electronic band structures (HSE) for the fully hydrogenated ZnSb monolayer sheet under strains of 0%, 4% and 8%, respectively. The Fermi level is set to zero.

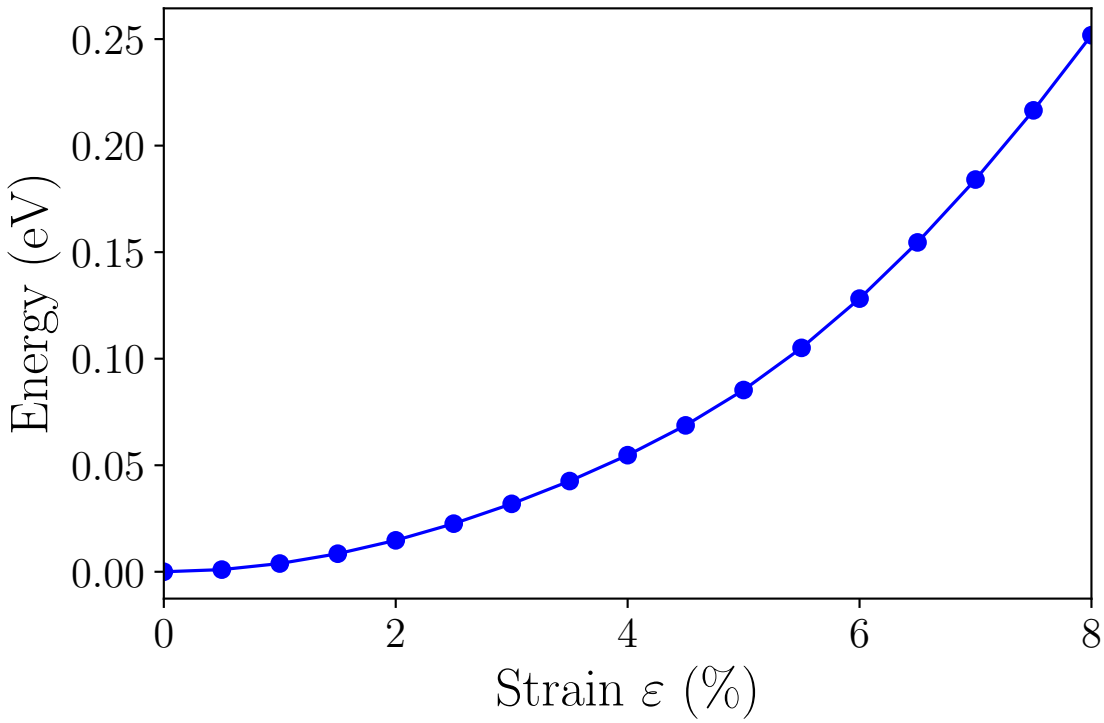

Figure S5. Total energy of the fully hydrogenated sheet as a function of strain. The total energy of the unstrained sheet is set to zero.