Electronic Supplementary Information

Exploration of Strain and Thermoelectric properties of hexagonal SiX (X = N, P, As, Sb, and Bi) monolayers

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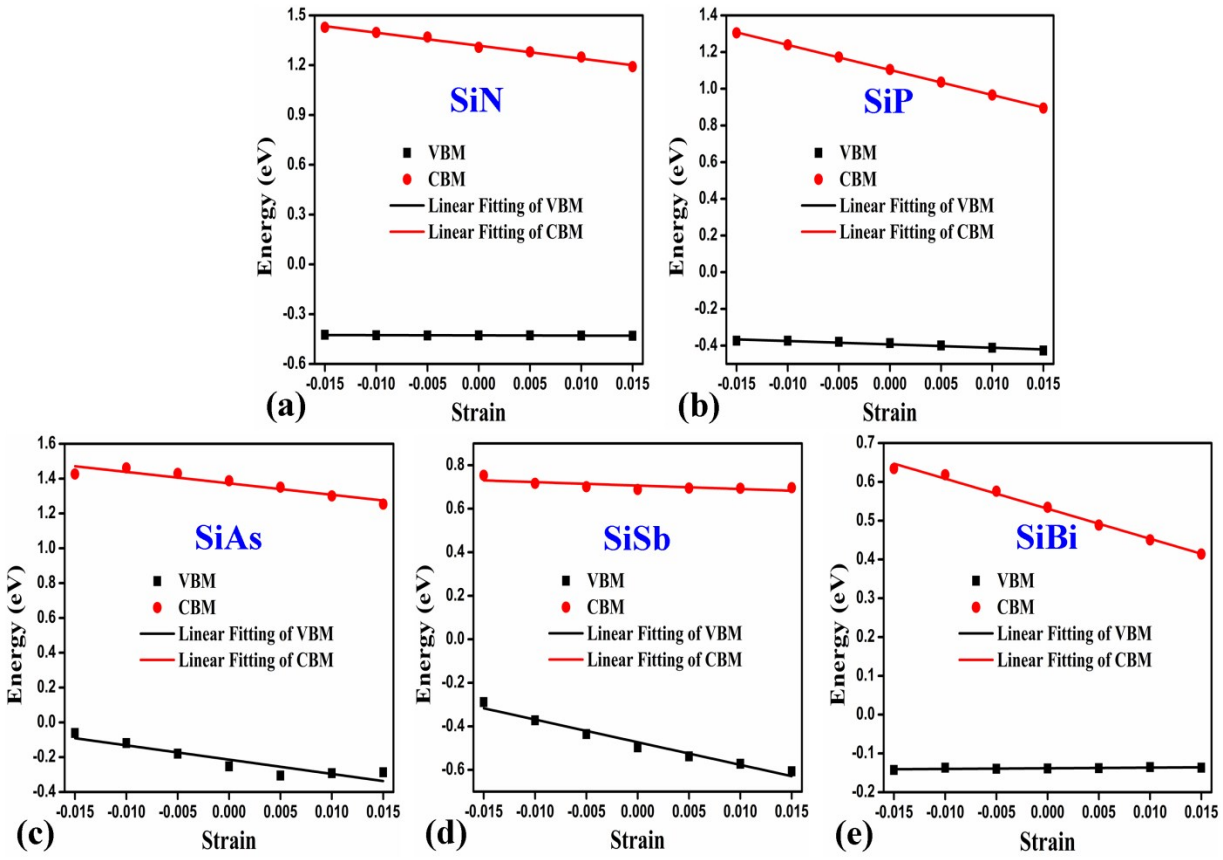


Fig. S1 Energy shift of VBM and CBM for monolayers (a) SiN, (b) SiP, (c) SiAs, (d) SiSb, and (e) SiBi w.r.t. compressive and tensile strains.

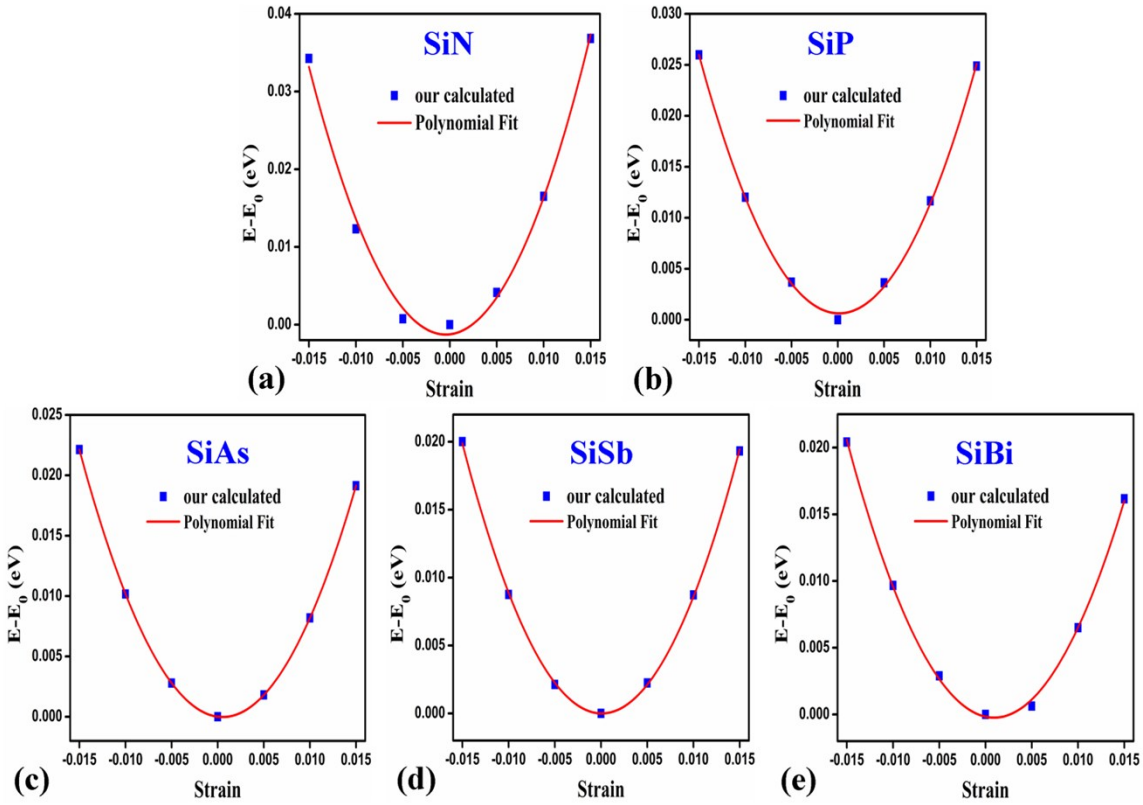
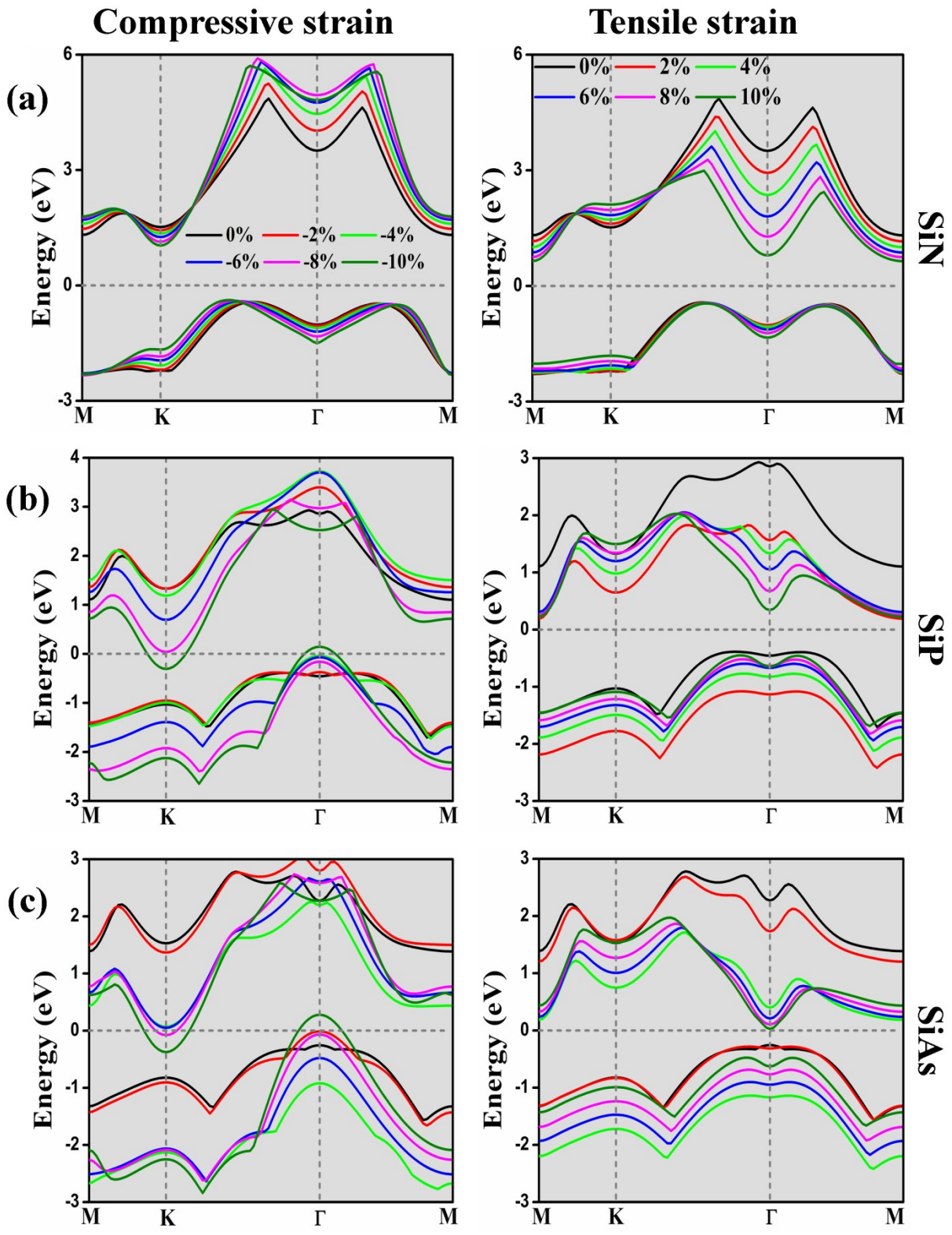


Fig. S2 Strain energy difference between the total energy of relaxed and applied biaxial strained monolayers (a) SiN, (b) SiP, (c) SiAs, (d) SiSb, and (e) SiBi w.r.t. compressive and tensile strains.


Compressive strain
Tensile strain
(a)
(b)
(c)
SiN
SiP
SiAs
Energy (eV)
0% -2% -4%
-6% -8% -10%
0% 2% 4%
6% 8% 10%
M K Γ M

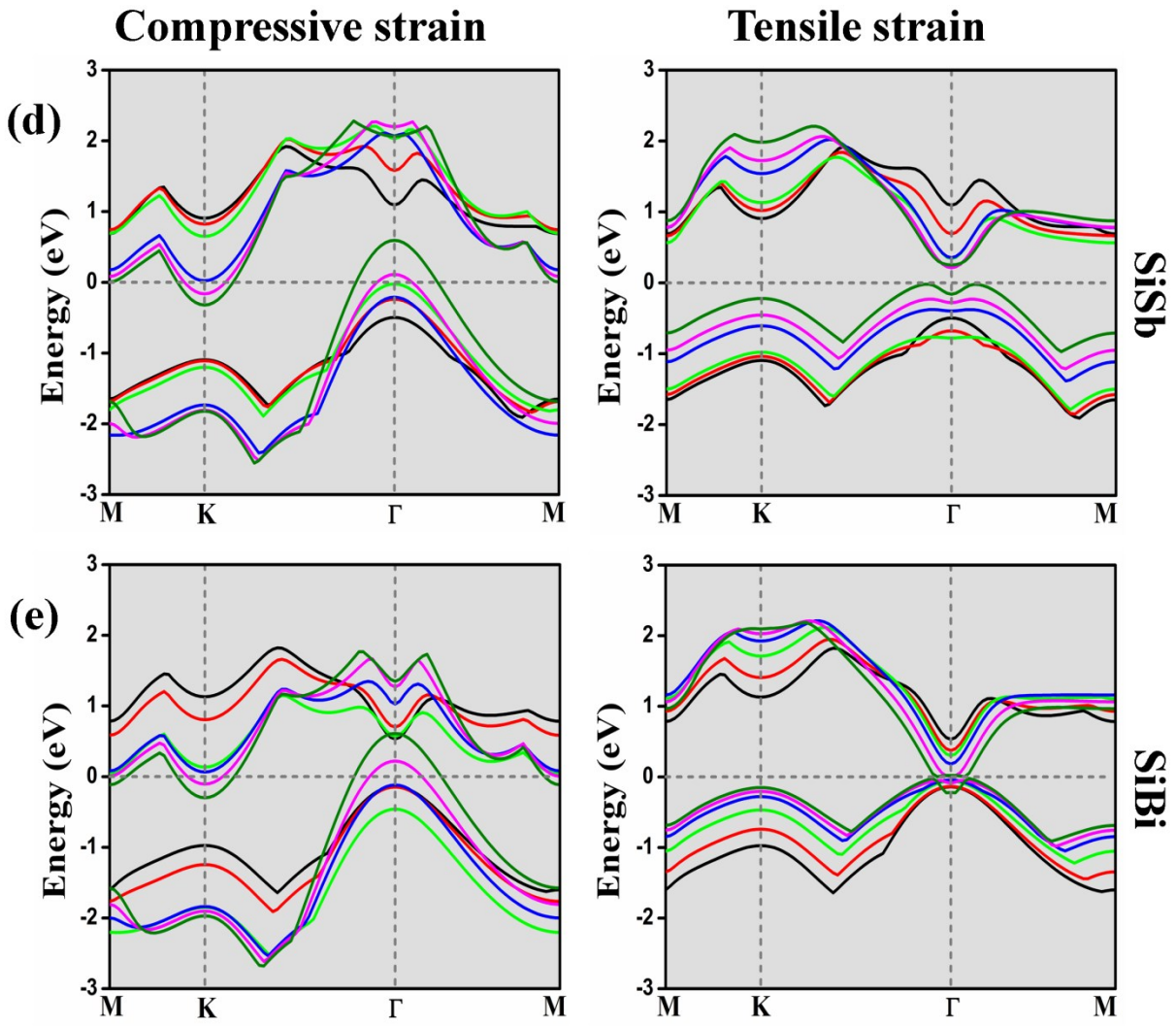


Fig. S3 Electronic band structures (a) SiN, (b) SiP, (c) SiAs, (d) SiSb, and (e) SiBi on application of compressive and tensile strain. The Fermi level is set at zero. The black, red, light green, blue, pink, and olive green colour indicates applied compressive or tensile biaxial strain of 0% (unstrained), 2%, 4%, 6%, 8%, and 10% respectively.

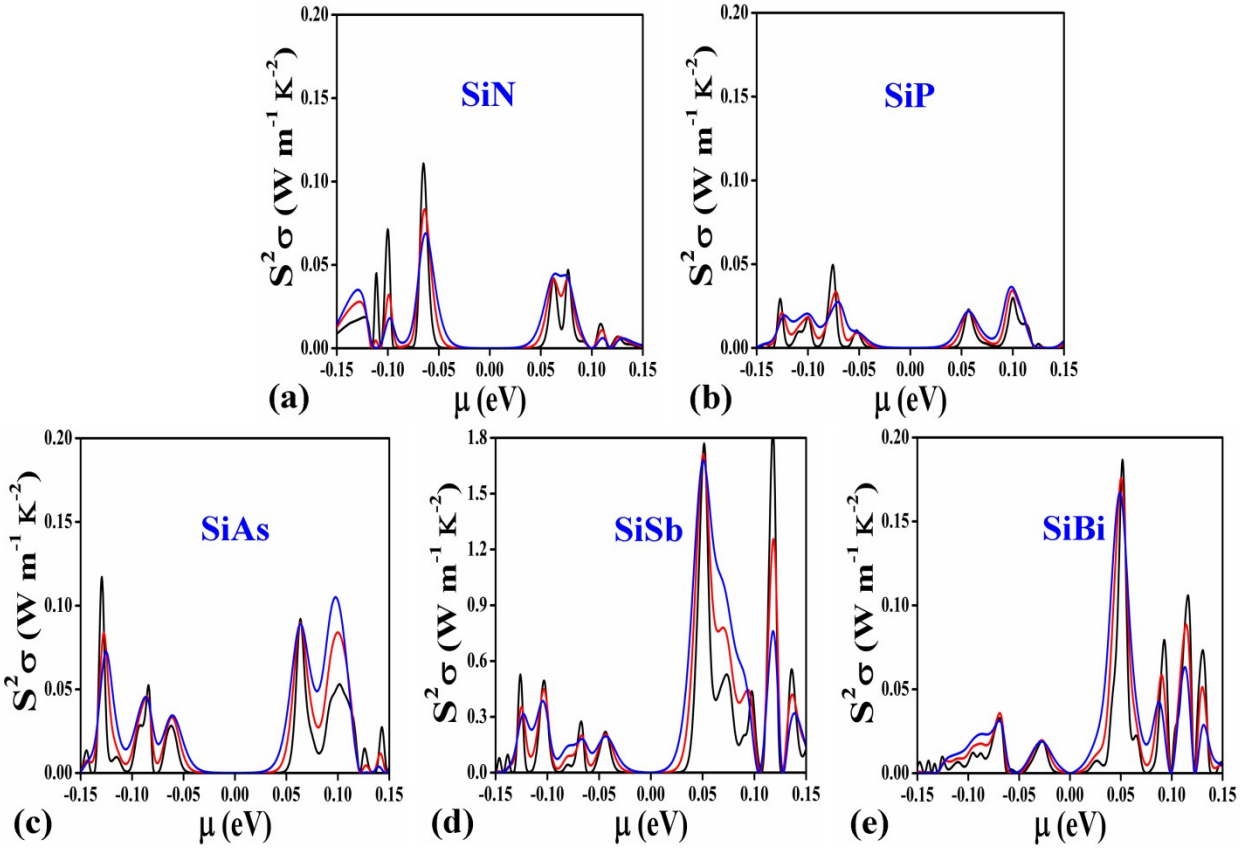


Fig. S4 The power factor plotted as a function of chemical potential at three different temperatures. The black, red, and blue lines indicate temperature values 300K, 500K, and 700K respectively.