Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Strain-induced enhancement in the electronic and thermal transport properties of Tin Sulphide bilayer

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August 31, 2021

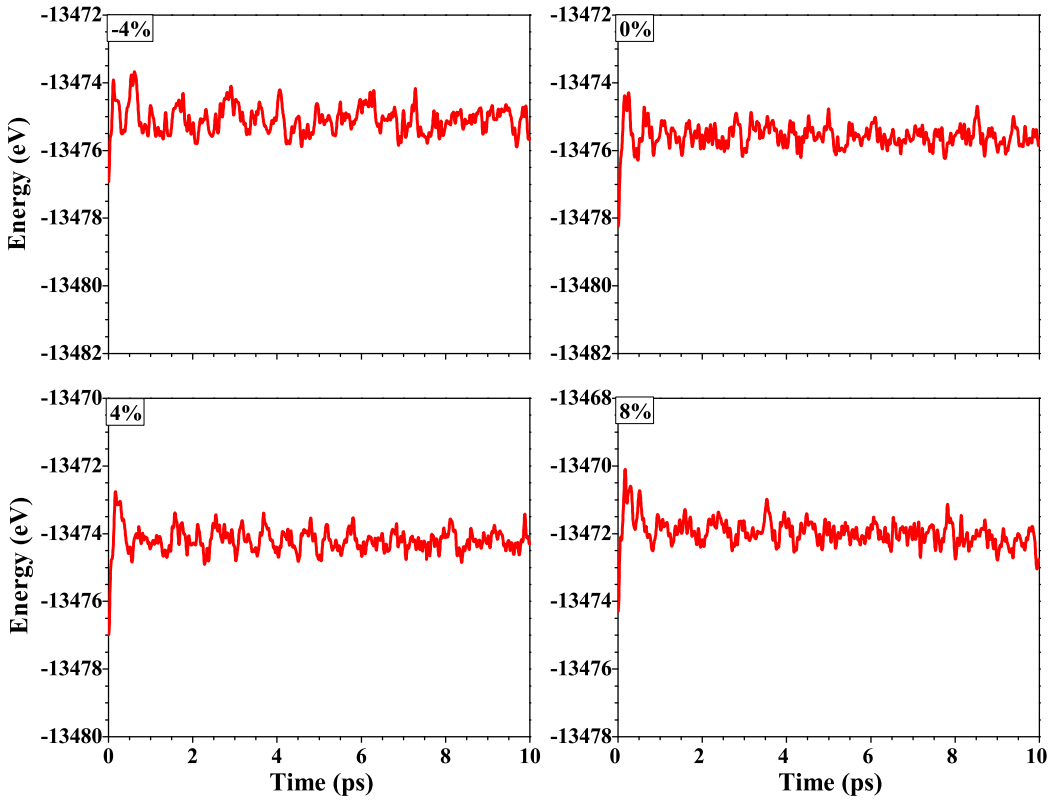

Figure 1 Energy fluctuations with respect to time at 300 K of SnS bilayer under different isotropic strains. Total energies remain almost invariant after heating for 10 pico-seconds which confirms the thermal stability of the SnS bilayers under different strains.

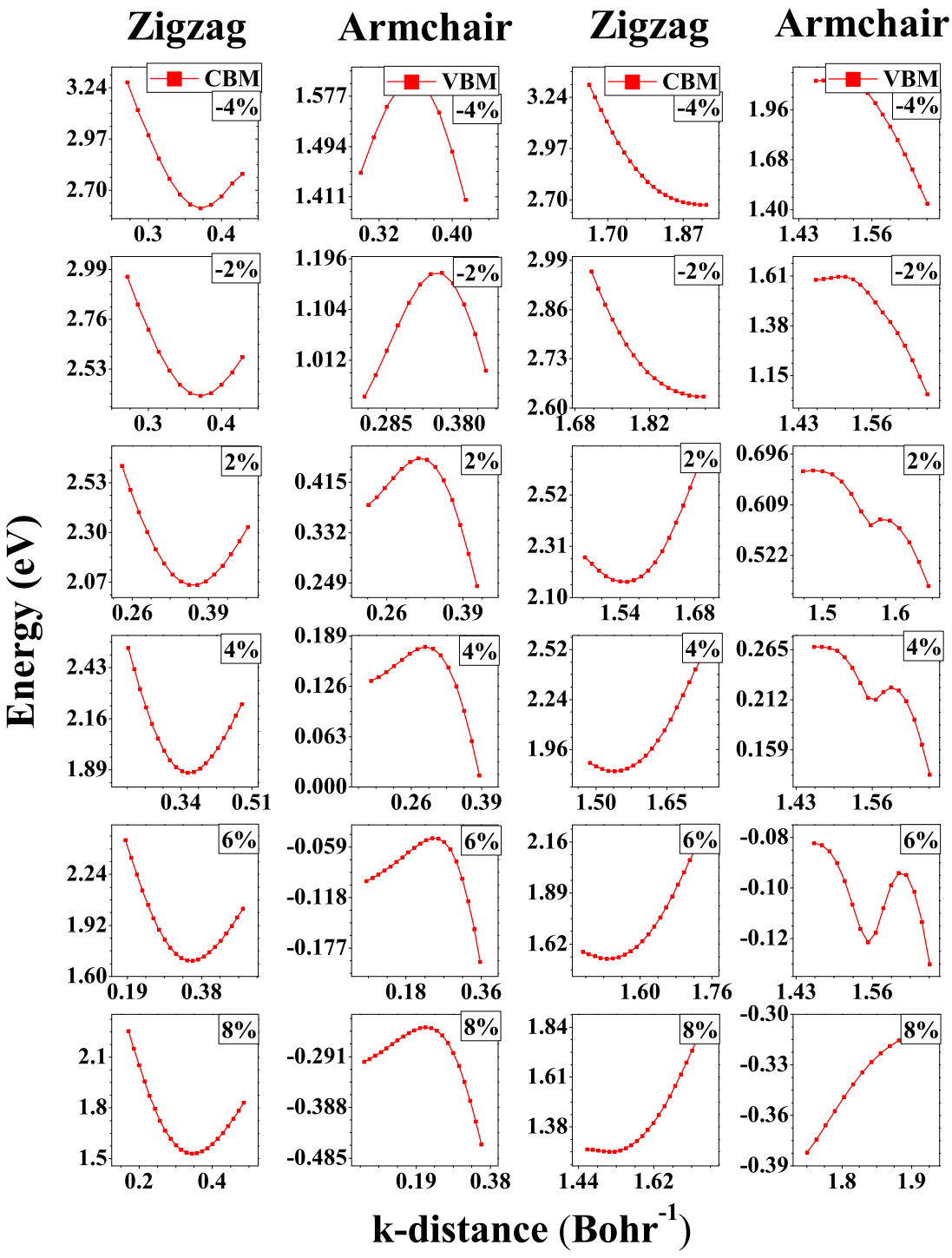

Figure 2 Effective mass (m^*) of charge carriers along zigzag and armchair directions of the SnS bilayer under different isotropic strains. The m^* of holes and electrons are calculated as, $m^*=\frac{\hbar^2}{\frac{\partial^2 E}{\partial k^2}}$, by fitting the VBM and CBM to a polynomial function.

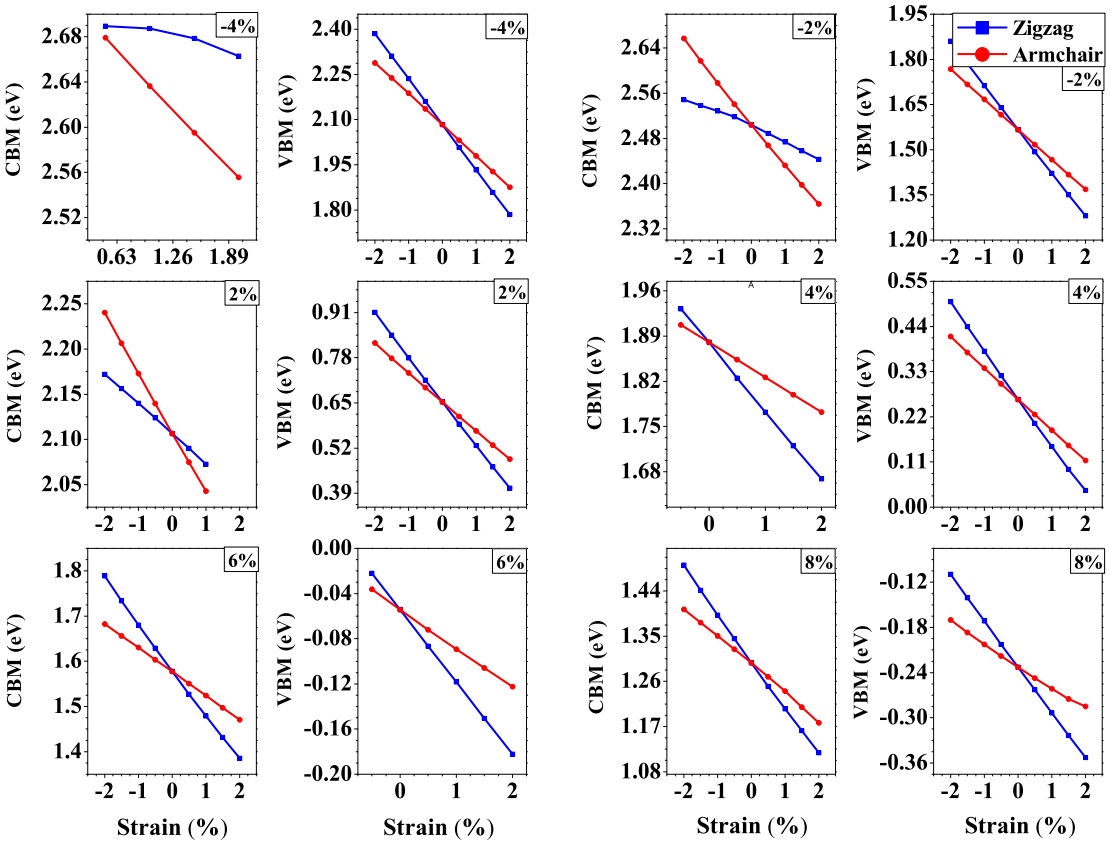

Figure 3 The energies of VBM and CBM as a function of uniaxial strain along the zigzag and armchair directions of the SnS bilayer under different isotropic strains. The slope of fitted straight line gives the value of E_β.

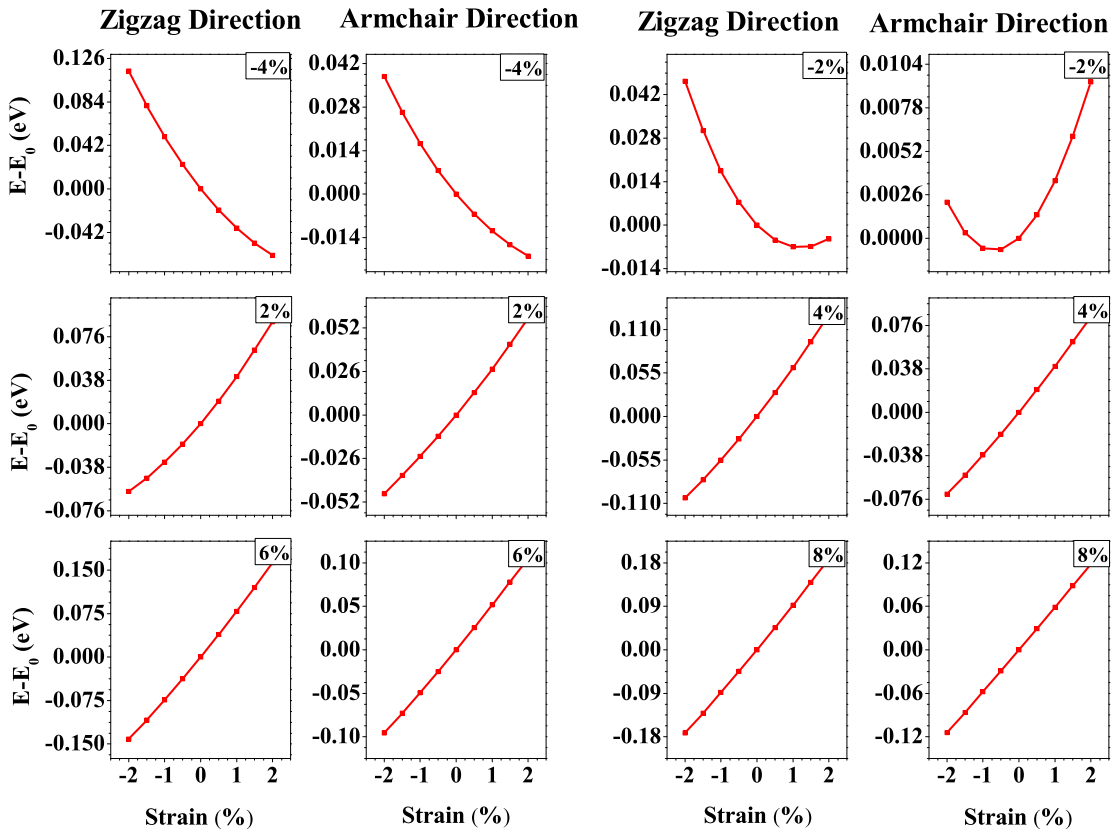

Figure 4 The change in total energy ($E - E_0$) as a function of uniaxial strain along the zigzag and armchair directions of the SnS bilayer under different isotropic strains. A quadratic polynomial fit to the curve gives the value of elastic constant (C_β).

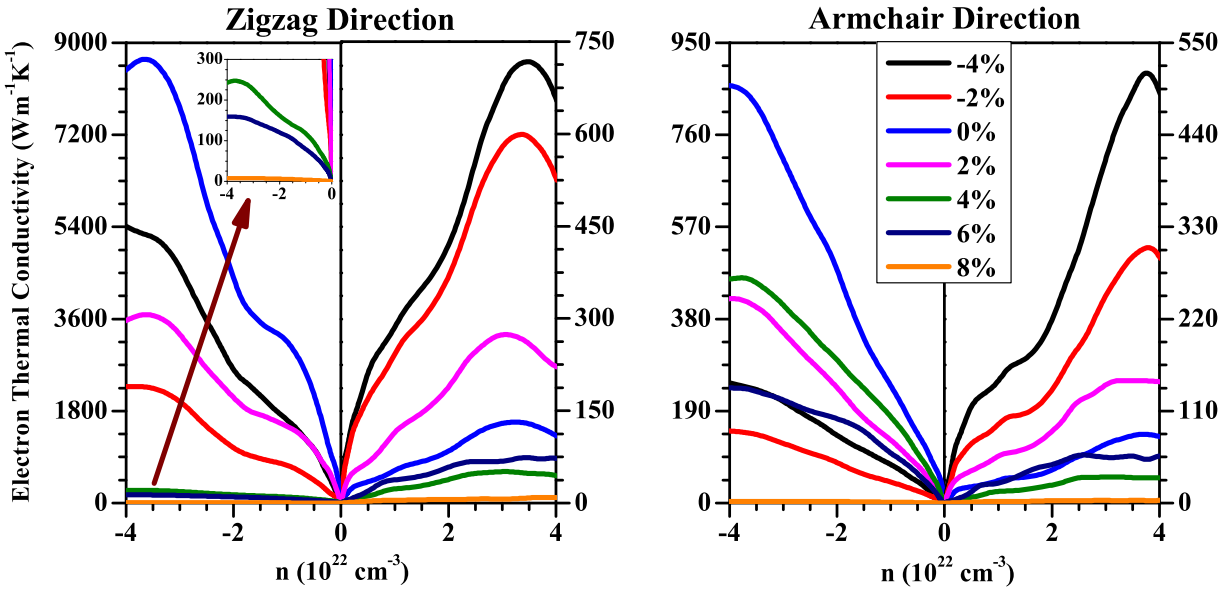

Figure 5 Room temperature electronic thermal conductivity (κ_e) as a function of n along the zigzag and armchair directions for the SnS bilayer under different isotropic strains. The κ_e has higher values for the n-type charge carrier concentration as compared to p-type charge carrier concentration due to the higher electron mobilities as compared to holes. The inset shows the behaviour of κ_e for the strain range 6-8%.