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Strain induced crystal lattice softening and improved thermoelectric performance of hydrogenated silicene for energy harvesting applications

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In recent years, Silicene has attracted great interest in various fields but does not fit well in the field of thermoelectrics due to the absence of electronic band gap. Nevertheless, hydrogenation of silicene (SiH) delocalize the free electrons and induces gap widening (2.19 eV), but its thermoelectric performance is still limited due to the larger band gap. Thermoelectric performance can be effectively improved using strain engineering, which allows modulation of crystal as well as electronic energy levels of a material. We studied the effect of biaxial tensile strain on structure, stability and thermoelectric properties of SiH monolayer. Taking clue regarding the stability from phonon dispersion, tensile strain upto 14% is incorporated and results are discussed. The distortion of crystal structure with strain manipulates the characteristics of electronic band structure such that there is an indirect to direct band gap transition along with decrease in band gap, effective mass and relaxation time of carriers. As a result, the Seebeck coefficient falls and attains minimum value at 14% strain while electrical conductivity and electronic thermal conductivity shows increasing trend and maximize at 14% strain. Another crucial consequence of strain is that tensile strain led to a considerable decrease in lattice thermal conductivity. At a strain of 14%, the lattice thermal conductivity at 700 K (0.28) decreased by approximately 43% compared to its unstrained counterpart (0.49 K), which is highly beneficial for achieving high ZT. To assess the efficiency of thermoelectric conversion, the ZT is computed, revealing an increase from 1.66 in the unstrained state to 2.83 at a strain of 14% and a temperature of 700 K. The calculations unveil a nearly twofold increase in ZT with the implementation of strain engineering, underscoring its effectiveness in augmenting the efficiency of thermoelectric devices.

Keywords Two-dimensional materials, Strain engineering, Phonon softening, First-principles calculations, Thermoelectric properties

To recover useless energy lost by different energy sources, people are seeking for efficient energy recovery techniques[1]. Many operations in both industries and daily life involve actions where a significant amount of energy is lost to the environment[2]. In the field of thermal management and energy harvesting, thermoelectric materials have attracted researchers as these materials assists in recovering the lost energy by utilising the Seebeck effect, the fundamental idea underpinning the conversion of heat into electricity[3]. The dimensionless figure of merit $ZT = \frac{S2\sigma T}{k}$, which includes Seebeck coefficient (S), electrical conductivity (σ) and total thermal conductivity ($k = k_l + k_e$) accurately quantify the efficiency of a thermoelectric material[4]. The parameters involved in ZT are inter-linked and challenging to individually adjust because of interdependency of S, σ and k, caused by carrier concentration. However, new ideas or techniques continue to enhance the thermoelectric performance

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