Supplemental Materials

Tailoring Electronic and Thermoelectric Properties of The SnSe Monolayer via Vacancy Defects: Insights from Density Functional Theory

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S1. k-point Convergence Test

To verify the reliability and accuracy of the DFT calculations, a k-point convergence test was carried out for the monolayer SnSe system. The total energy was calculated using different Monkhorst–Pack grids ranging from $2 \times 2 \times 1$ to $10 \times 10 \times 1$. As shown in Figure S1, the variation of total energy becomes negligible beyond the $7 \times 7 \times 1$ grid, where the difference in total energy compared to $8 \times 8 \times 1$ is less than 1 meV/atom. Therefore, the $7 \times 7 \times 1$ k-point grid was selected for all subsequent calculations of perfect and defected SnSe monolayers to ensure a good balance between computational accuracy and efficiency.

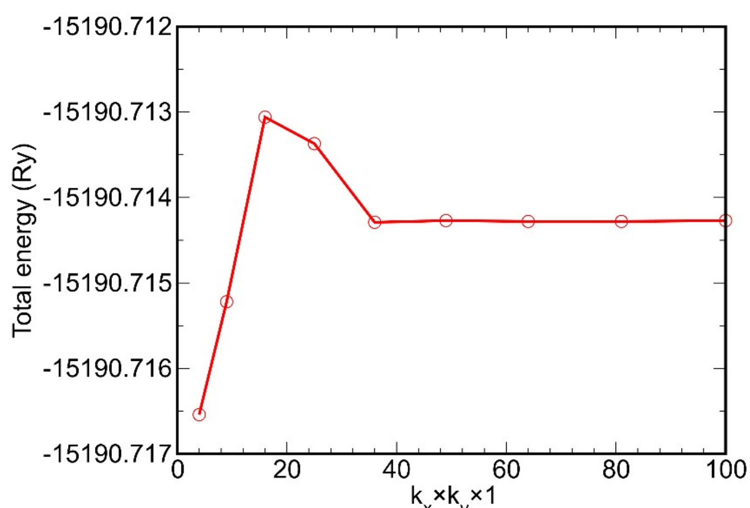

Figure S1. Total energy (in Ry) of the SnSe monolayer as a function of k-point mesh density ($k_x \times k_y \times 1$) obtained using the Monkhorst–Pack scheme. The total energy becomes nearly constant beyond the $7 \times 7 \times 1$ grid, indicating convergence of the Brillouin zone sampling.

S2. Normalized Transport Coefficients.

To complement the discussion of thermoelectric transport properties, the normalized electrical conductivity (σ/τ) and electronic thermal conductivity (κ_e/τ) were calculated as functions of the chemical potential (μ_{chem}) for all monolayer systems (SnSe, $Sn_{0.94}$Se, $SnSe_{0.94}$, and $Sn_{0.94}Se_{0.94}$) at 300 K. These quantities allow the intrinsic electronic transport behavior to be analyzed without the influence of the absolute value of relaxation time (τ) derived from potential deformation theory. The σ/τ and κ_e/τ curves exhibit consistent trends, indicating that the variations in electrical and electronic thermal transport are primarily governed by the electronic structure modifications induced by vacancies. Furthermore, the correlation between σ/τ and κ_e/τ confirms that the Wiedemann–Franz relationship remains valid across all considered systems.

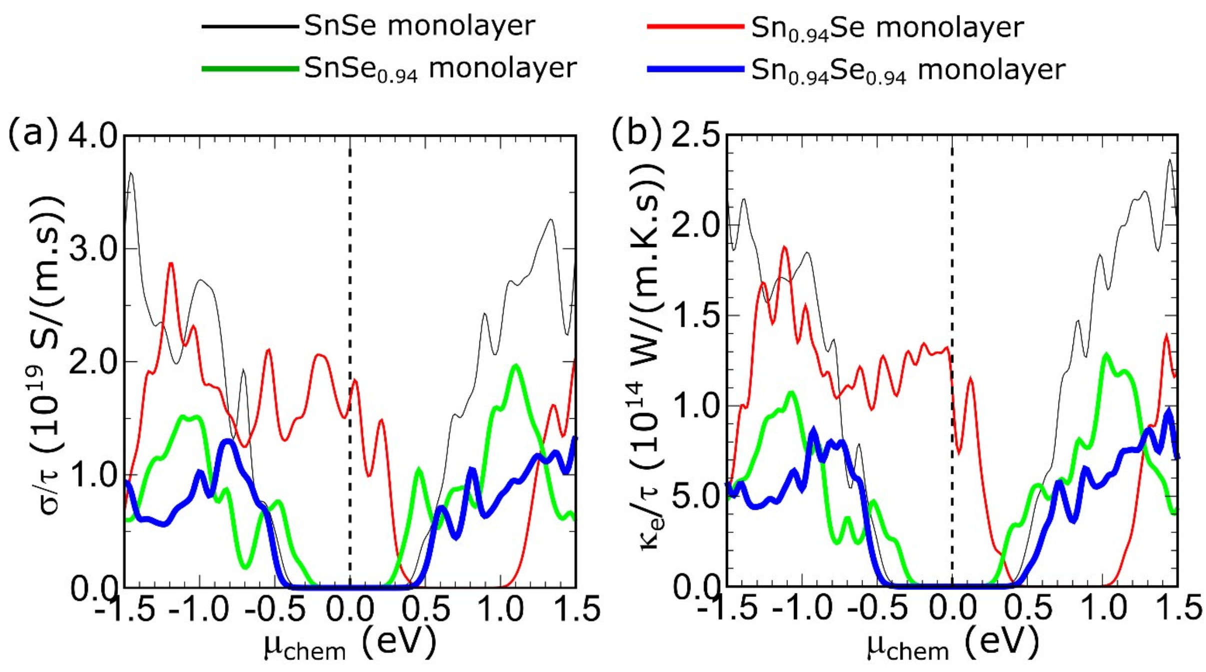

Figure S2. Normalized (a) electrical conductivity (σ/τ) and (b) electronic thermal conductivity (κ_e/τ) as a function of μchem for the SnSe, $Sn_{0.94}$Se, $SnSe_{0.94}$, and $Sn_{0.94}Se_{0.94}$ monolayers at 300 K.