

Supplementary Information

Electron-Phonon interaction effect in the photovoltaic parameters of indirect (direct) bandgap AlSb (GaSb) p-n junction solar cell devices: An *ab-initio* quantum mechanical study

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S-I. Special thermal displacement (STD) method

It can be shown that the average transmission from a thermal distribution of configurations describes the inelastic electron transmission spectrum due to electron–phonon scattering with reasonable accuracy [31]. In the special thermal displacement (STD) method, a single representative configuration is used instead of the average. The STD method is quite advantageous as it reduces the computational cost of inelastic transport calculations significantly. The STD configuration is obtained by calculating the phonon eigenfunctions and eigenvalues first using the dynamical matrix of the central region. The STD vector of atomic displacements is expressed as:

$$\vec{u}_{\text{STD}}(T) = \sum_{\lambda} S_{\lambda} (-1)^{\lambda-1} \vec{e}_{\lambda} \sigma_{\lambda}(T) \quad (\text{S-I-1})$$

The phonon modes are labelled by λ with eigenmode vector e_{λ} , frequency ω_{λ} , and characteristic length l_{λ} . S_{λ} denotes the sign of the first non-zero element in e_{λ} . S_{λ} enforces the same choice of gauge for the modes. The σ is the Gaussian width and is related to the mean square displacement as:

$$\langle \vec{u}_{\lambda}^2 \rangle = l_{\lambda}^2 \left(2n_B \left(\frac{\hbar\omega_{\lambda}}{k_B T} \right) + 1 \right) = \sigma_{\lambda}^2(T) \quad (\text{S-I-2})$$

The T and n_B are the temperature and the Bose–Einstein distribution, respectively. The STD method exploits the use of opposite phases for phonons with similar frequencies. This results in the average phonon–phonon correlation functions vanishing. Further, the transmission spectrum of the STD configuration becomes similar to a thermal average of single phonon excitations. Finally, the Hamiltonian of the system displaced by \vec{u}_{STD} is calculated self-consistently followed by the calculation of the transmission spectrum.

S-II: Non-equilibrium Green Function (NEGF) method

In NEGF method [31], the electron density is expressed in terms of the electron density matrix that is split into left and right contributions.

$$D = D^L + D^R \quad (\text{S-II-1})$$

The left contribution is computed as:

$$D^L = \int \rho^L(\varepsilon) f\left(\frac{\varepsilon - \mu_L}{k_B T_L}\right) d\varepsilon \quad (\text{S-II-2})$$

$$\rho^L(\varepsilon) \equiv \frac{1}{2\pi} G(\varepsilon) \Gamma^L(\varepsilon) G^\dagger(\varepsilon) \quad (\text{S-II-3})$$

where $\rho^L(\varepsilon)$ is the spectral density matrix given in terms of the retarded Green's function G and the broadening function Γ^L of the left electrode,

$$\Gamma^L = \frac{1}{i} \left(\Sigma^L - (\Sigma^L)^\dagger \right) \quad (\text{S-II-4})$$

The broadening function Γ^L is given by the left electrode self-energy Σ^L . The central region has a non-equilibrium electron distribution. However, the electron distribution in the left electrode is given by a Fermi–Dirac distribution $f_L(\varepsilon)$ with an electron temperature T_L . The right density matrix contribution is also given by similar equations.

S-III: Phonon calculations

The phonon modes and eigenfunctions of the system (molecular or periodic), can be calculated by computing and thereby diagonalizing the dynamical matrix (D)^[35]. In case of small thermal displacements of atoms around their equilibrium position, the harmonic approximation can be used. Within the harmonic approximation, the vibrational frequencies of a configuration are eigenvalues of the dynamical matrix D

$$D_{a,\alpha; b,\beta} = \frac{dF_{b,\beta}}{\sqrt{m_a m_b} dr_{a,\alpha}}$$

where m_a (m_b) is the atomic mass of atom a (b) and $dF_{b,\beta}/dr_{a,\alpha}$ is the force constant. The dynamical matrix can be calculated using finite difference (FD) method. In this method each matrix element is computed by displacing atom a along Cartesian direction α , and then calculating the resulting forces on atom b along directions β . This approach is sometimes referred to as the frozen-phonon or supercell method,

In the present article, the inter-atomic interactions between atoms described using generalized self-consistent force field potentials developed by Tersoff^[35, 39]. The unit cell is optimized with force field potential till the force on each atom is reduced to less than 0.001 eV/Å and stress tolerance is reduced to 0.0001 eV/Å³. This optimized crystal structure is used to calculate the dynamical matrix, which in turn is used for compute the phonon band structure and phonon density of states.