Supporting Information for

External electric field driving ultra-low thermal conductivity of silicene

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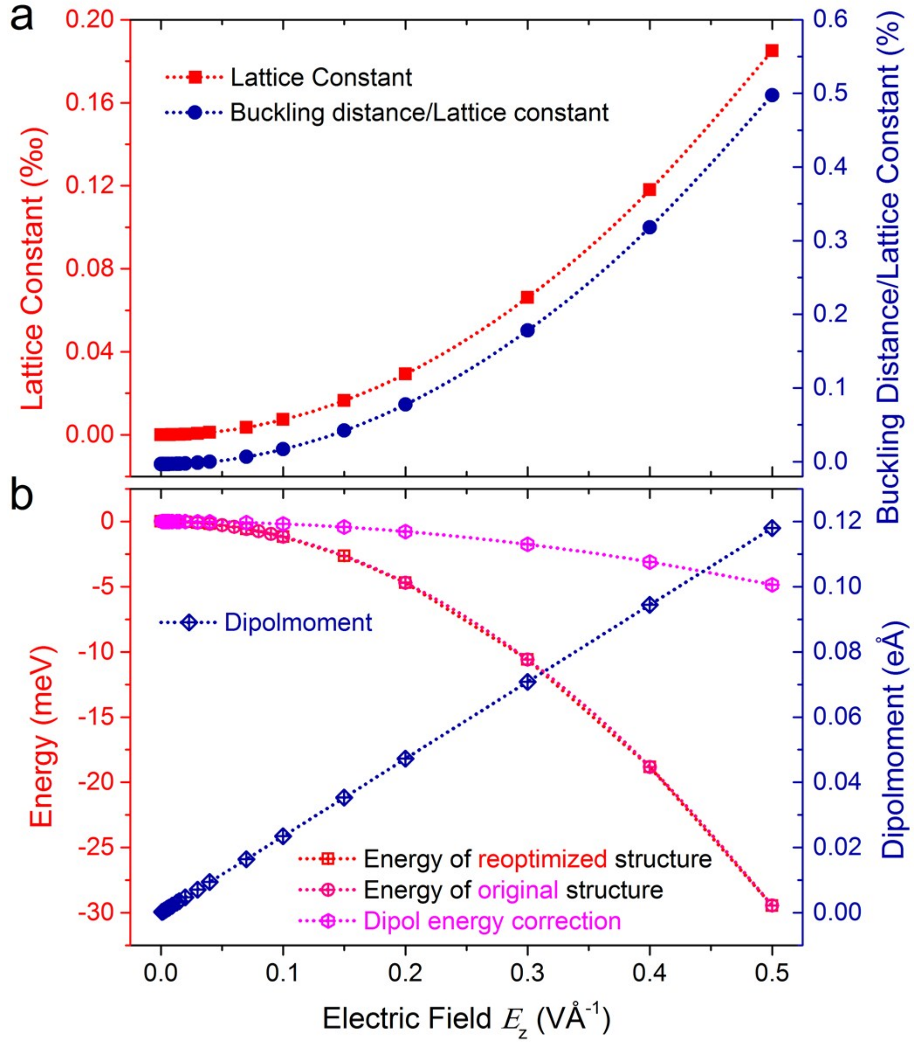

FIGURE S1. Effect of electric field on geometry structure and energy of silicene. (a) The relative lattice constant and buckling distance (lattice constant) with respect to E_z. (b) The energy (left axis) and the dipolmoment (right axis) *vs*. E_z. The results obtained without re-optimizing the atomic structure are also plotted for comparison.

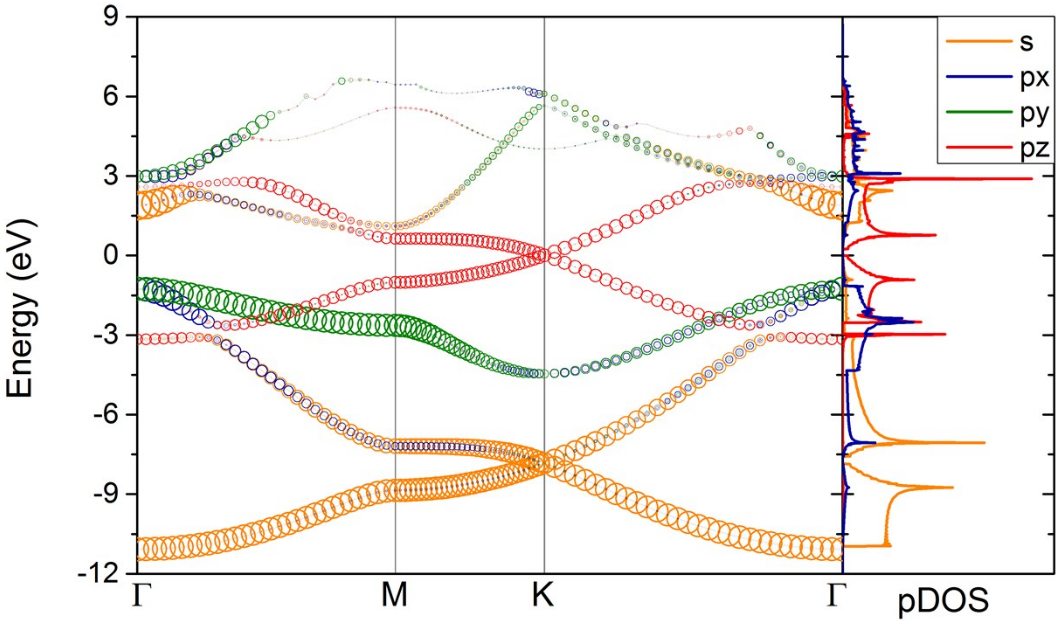

FIGURE S2. The orbital-projected band structures and density of states (pDOS) of silicene without external electric field. The Dirac cone is mainly contributed by the p_z orbital of Si atoms.

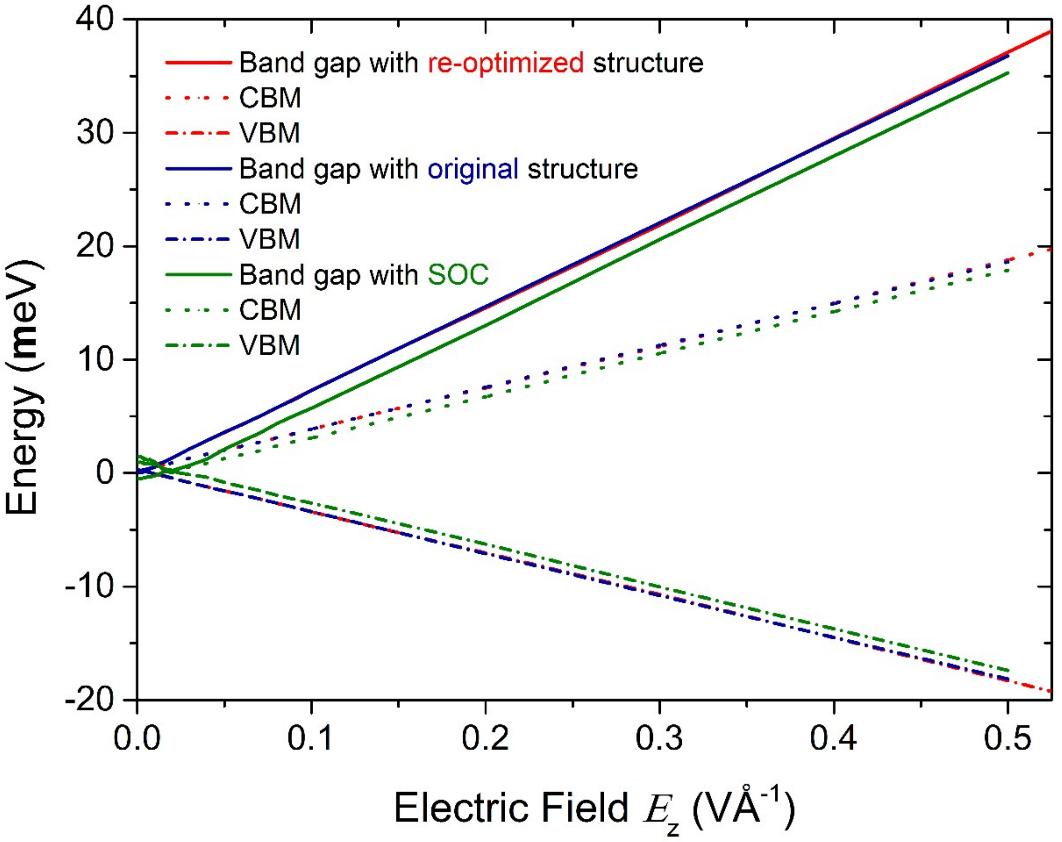

FIGURE S3. Comparison of energy band gap, conduction band minimum (CBM) and valence band maximum (VBM) as a function of E_z with and without considering the spin-orbital couplings (SOC). The results obtained without re-optimizing the atomic structure are also plotted for comparison.

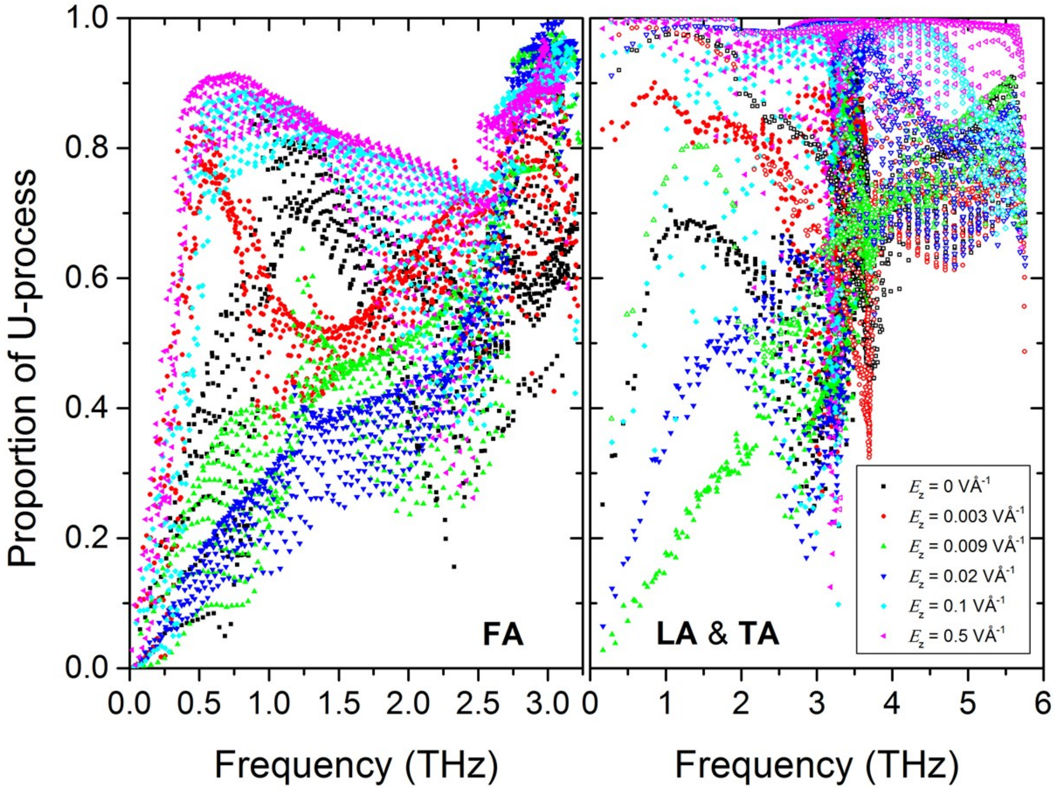

FIGURE S4. The proportion of U-process in the total scattering rate of acoustic phonon modes (left, FA; right, LA and TA) for some representative cases of external electric fields.

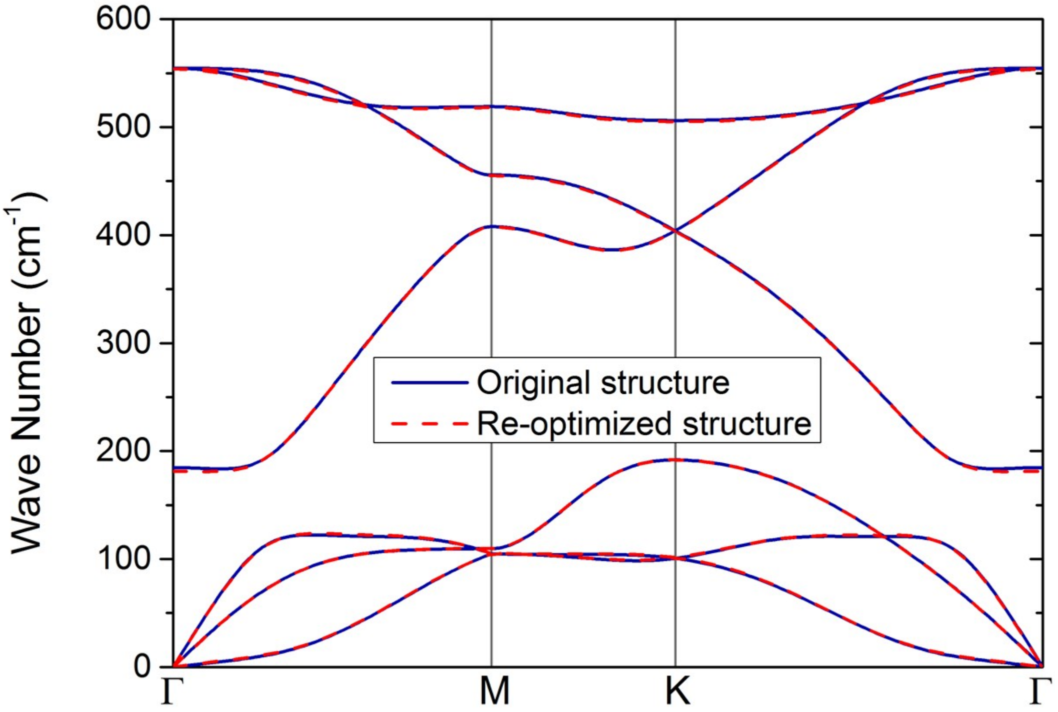

FIGURE S5. The comparison of phonon dispersions of silicene using the original and re-optimized structures for electric field of 0.5 VÅ^{-1}. The original structure means that the optimized structure with no electric field was used for calculating the phonon dispersions. The re-optimized structure is the fully optimized structure with electric field applied. Both the phonon dispersions are calculated with the electric field of 0.5VÅ^{-1} applied.

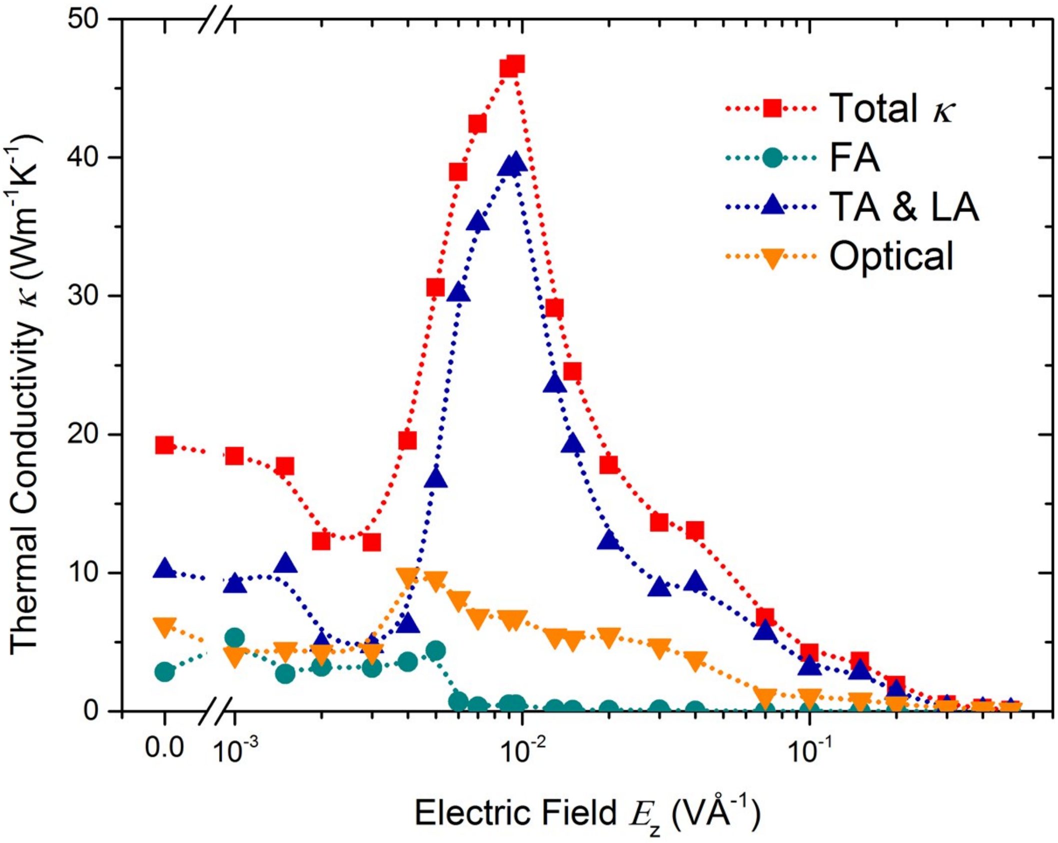

FIGURE S6. The contribution from different phonon branch to the overall thermal conductivity *vs.* electric field.

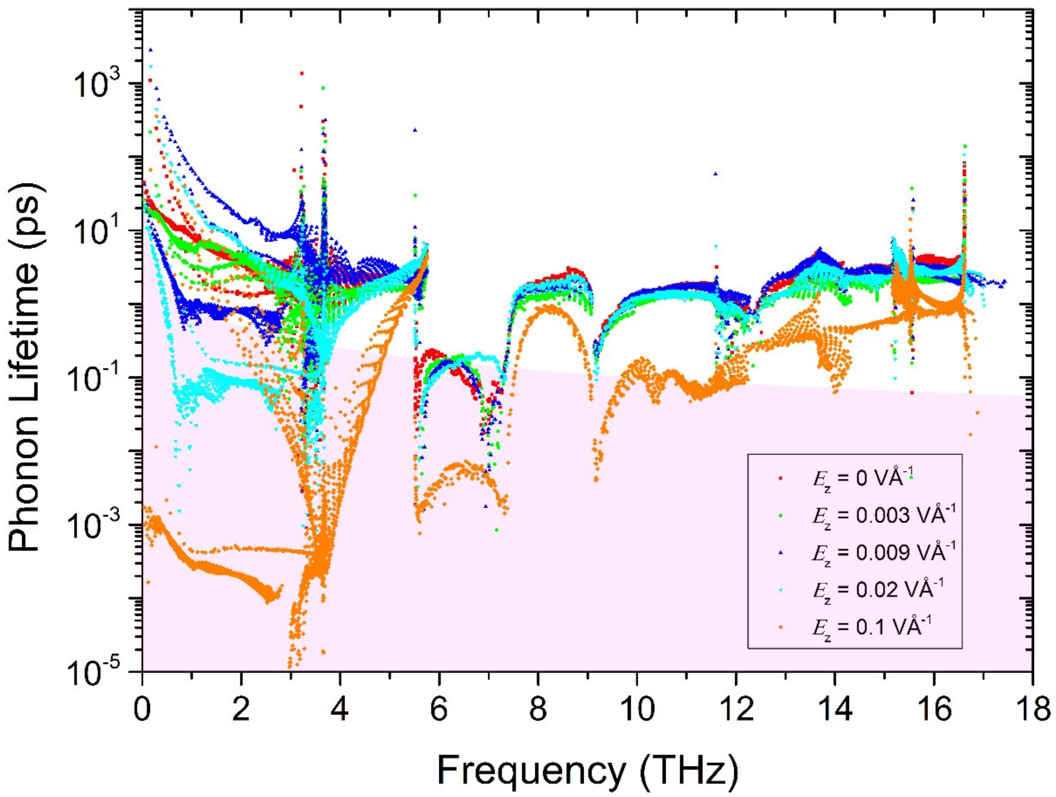

FIGURE S7. Phonon lifetime for the cases of representative electric fields. The colored area indicates strongly scattered phonons beyond the Ioffe-Regel limit.

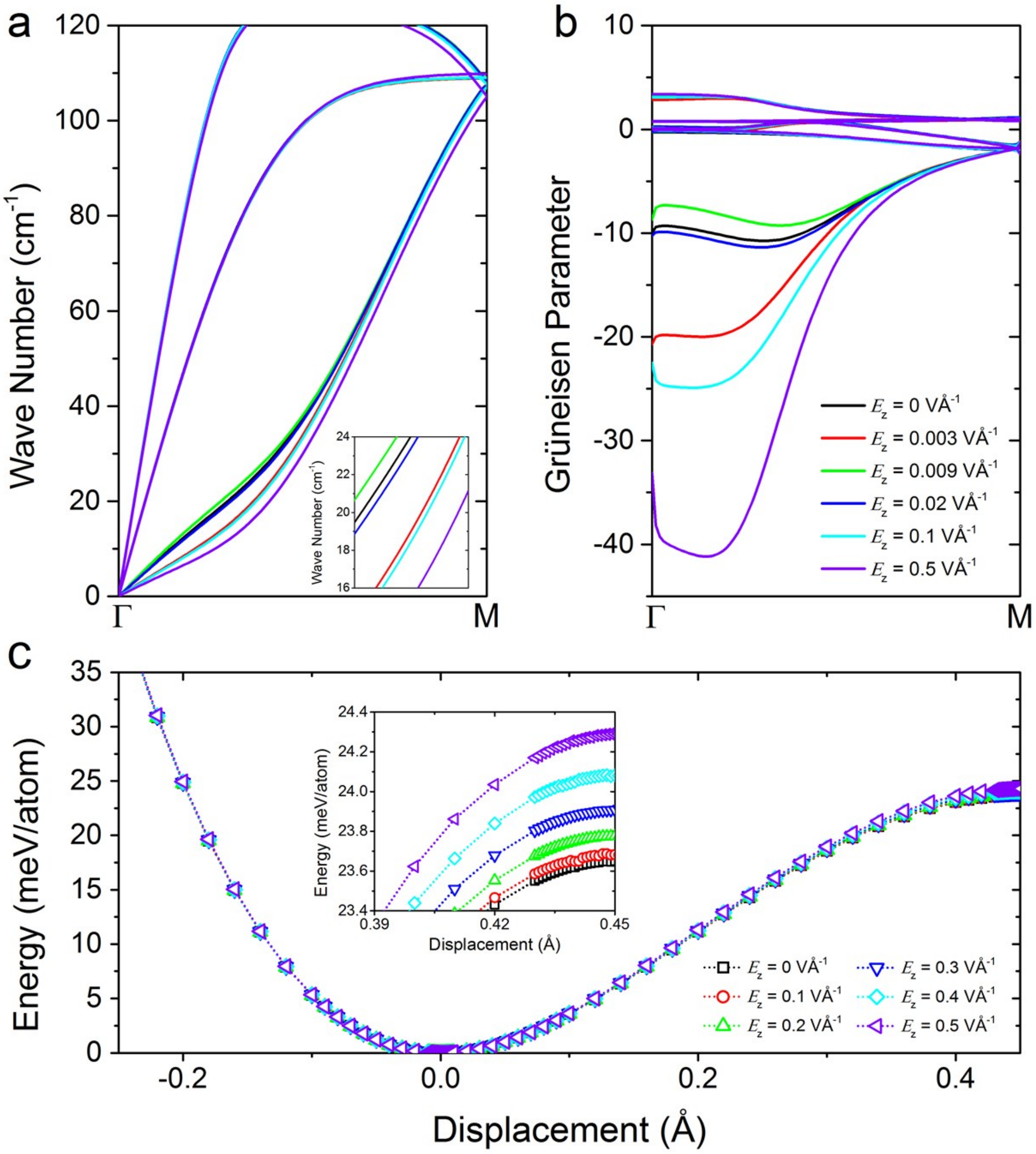

FIGURE S8. Electric field modulated phonon anharmonicity. (a) Phonon dispersion and (b) Grüneisen parameter along Γ-M of silicene for some representative electric fields. (Inset) Zoom-in of 30%-40% region of Γ-M. (c) Potential energy change per atom with respect to displacement of Si atom (sublattice-B) along the *out-of-plane* direction. (Inset) Zoom-in of the potential energy change near the displacement of 0.42 Å.

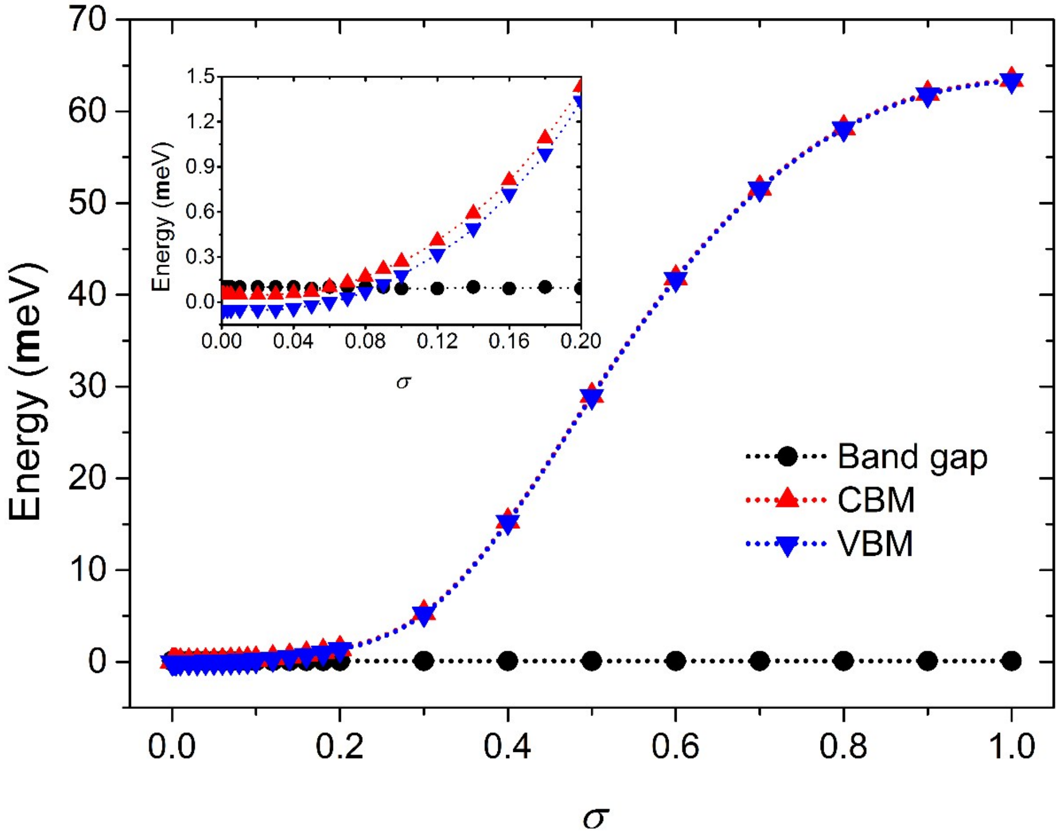

FIGURE S9. The effect of σ, which has the similar effect as finite temperature, on the energy band gap, the relative position to Fermi energy (chemical potential) of conduction band minimum (CBM) and valence band maximum (VBM). (Inset) Zoom-in of the energy with small σ.

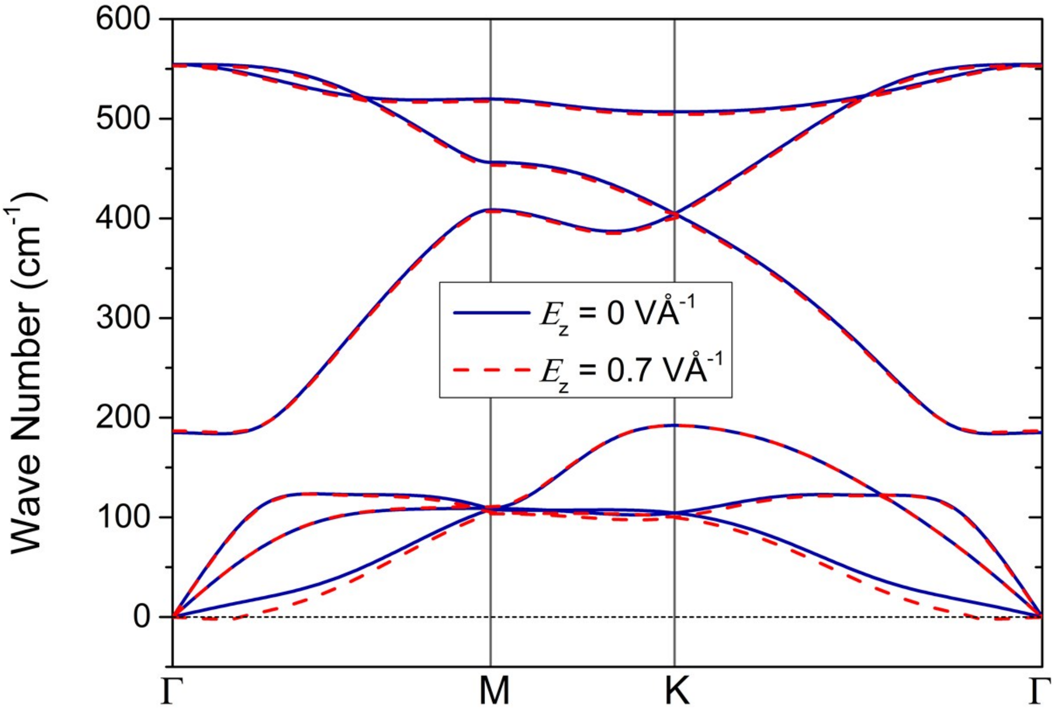

FIGURE S10. The comparison of phonon dispersions of silicene with and without electric field applied (0.7 VÅ^{-1}). Silicene structure will be thermodynamically unstable (evidenced by the imaginary frequencies) when the electric field of 0.7 VÅ^{-1} is applied.

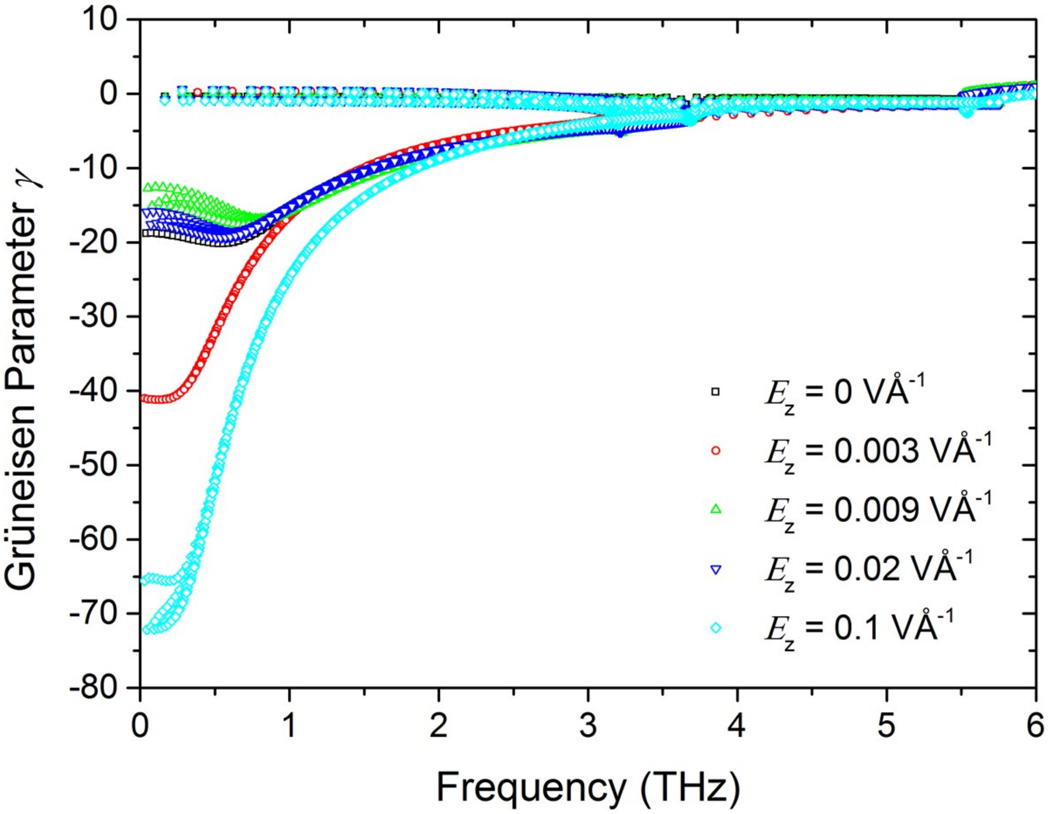

FIGURE S11. Comparison of mode level Grüneisen parameter of silicene among several representative electric fields. The results obtained from ShengBTE package are consistent with that obtained from PHONOPY package (Fig. S7).

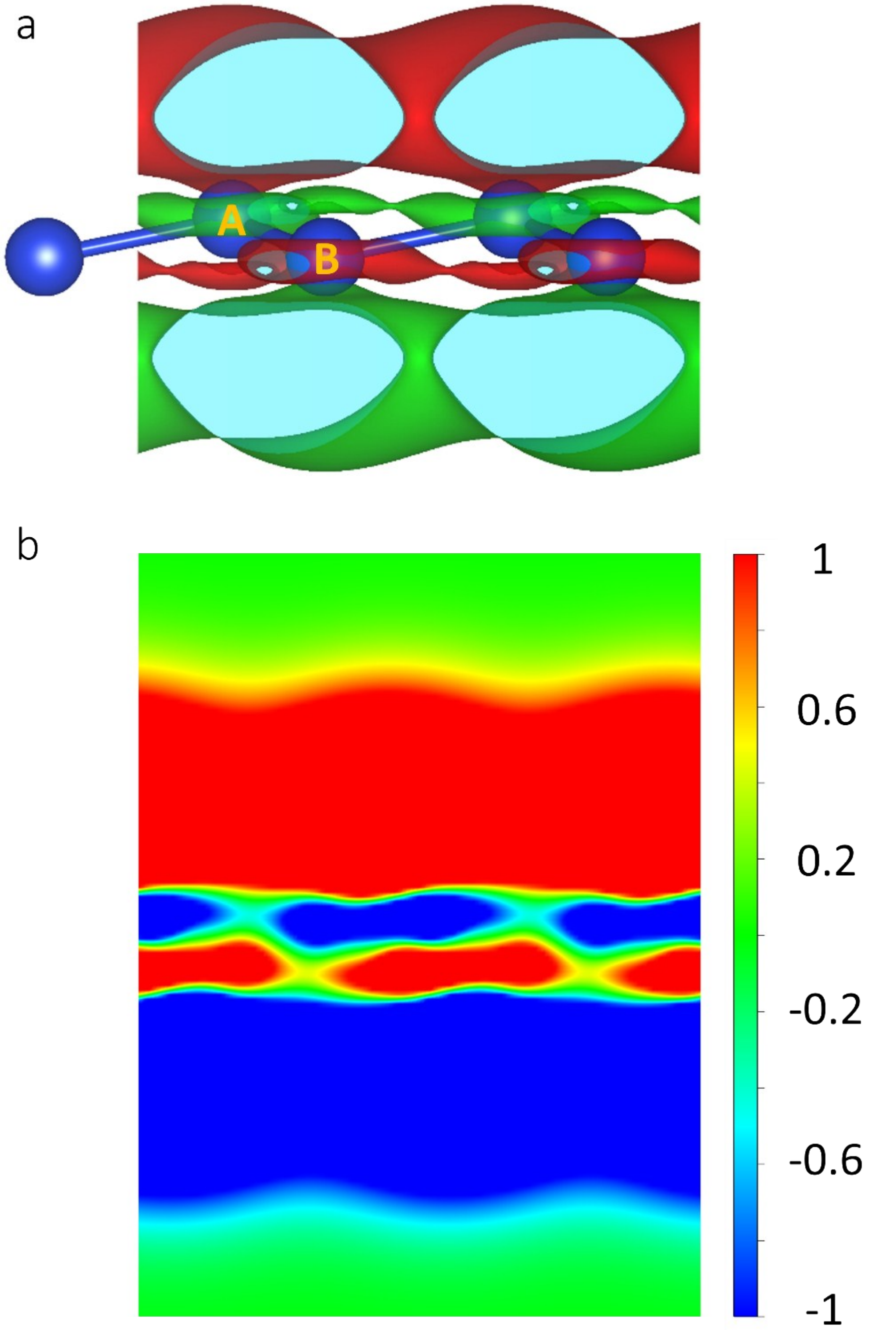

FIGURE S12. The electric field modulated charge environment. (a) The induced charge density ($\Delta\rho = \rho(E_z = 9\ \mathrm{mV\AA^{-1}}) - \rho(E_z = 0)$, isosurface level: 1.5×10^{-6}; red: positive accumulation of charge, green: negative depletion of charge). The Si atoms located at different sublattices are labeled on site as "A" and "B", respectively. (b) The projection of induced charge density in the unit of $1.64\ \times10^{-5}\ \mathrm{e\AA^{-3}}$.

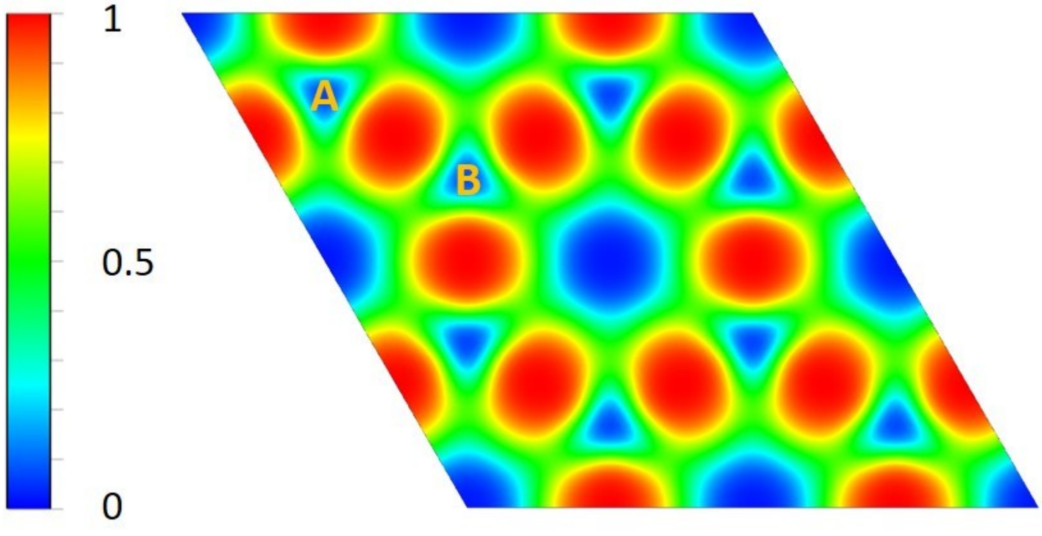

FIGURE S13. The electron localization functions (ELF) of silicene without external electric field. The positions where Si atoms locate in different sublattices are labeled on site as A and B, respectively.