Electronic Supplementary Information (ESI)

SiC_7 Siligraphene: Novel Donor Material with Extraordinary Sunlight Absorption

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More computational details

The first-principle molecular dynamics (FPMD) simulation was carried out with constant temperature and constant volume ensemble (NVT). The temperature was set 2000, 3000, and 3500 K respectively. The total simulation time of 5 ps was carried on with time step of 1.0 fs. The Nose algorithm[1] was used for temperature control. The optimized g-SiC_7 4×4 supercell was used as the initial structure. The phonon calculations were carried out by using the finite displacement method as implemented in the PHONOPY code.[2]

To compare the stability of the g-SiC_7 with other graphene-like 2D materials, the binding energy (E_b) was calculated as

$$E_b = (xE_{Si} + yE_C - E_{SixCy})/(x + y)$$

In this definition, E_{Si}, E_C, and E_{SixCy} repersent the energies of Si atom, C atom, and Si_xC_y nanomaterial, respectively. The larger binding energy, the more stable the structure is.

Absorbance calculations

The interband optical transition is relevant with the imaginary part of the dielectric tensor $\epsilon_2(\omega)$, which is a function of photon frequency ω. The monolayer absorbance $A(\omega)$ of the 2D materials, which is defined as the fraction of photon energy ($E = \hbar\omega$) adsorbed by the monolayer, is calculated using the following approximation:[3, 4]

$$A(\omega) = \frac{\omega}{c}\epsilon_2(\omega)\Delta z$$

Here c is the speed of light, and Δz is the size of the simulated cell in the layer-normal direction. This formula can be viewed as a Taylor expansion for small thickness Δz of the absorbance $A = 1 - e^{-\alpha \cdot \Delta z}$ for a flat layer of a bulk material with thickness Δz and absorption coefficient $\alpha = \frac{\epsilon_2(\omega)}{cn}$, with refractive index n = 1 due to the presence of vacuum in the vast majority of the simulation cell. Equivalently, it can be seen as deriving from the polarizability per unit area.

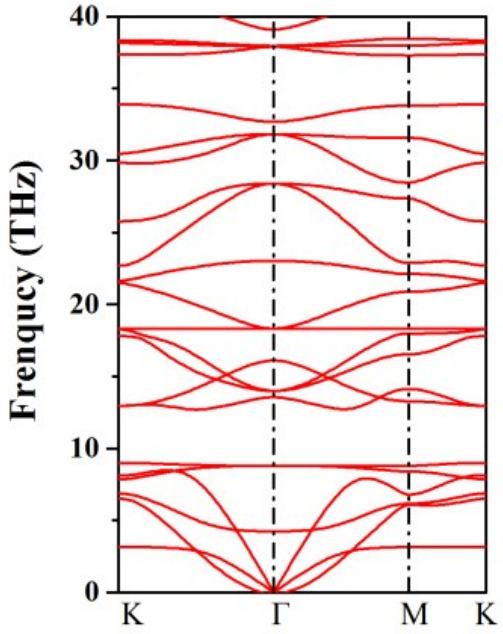

Fig. S1 The phonon dispersion of g-SiC_7 siligraphene. Γ, K and M correspond to the (0, 0, 0), (0.333, 0.666, 0) and (0, 0.5, 0) k-points in the first Brillouin zone (BZ),

respectively.

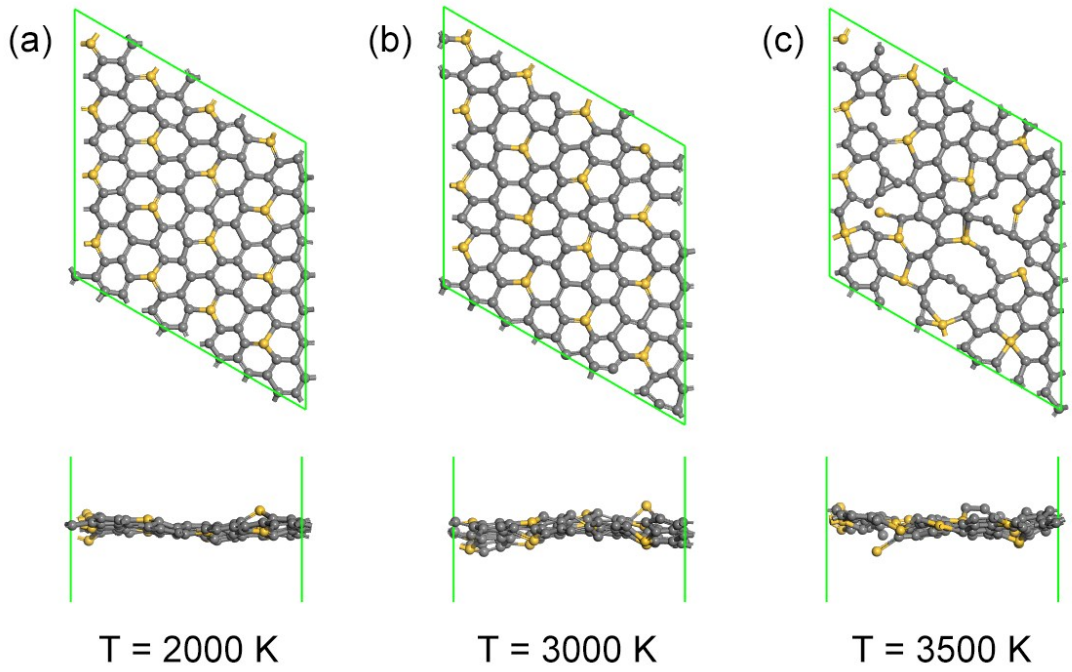

Fig. S2 Snapshots of the g-SiC_7 4×4 supercell at temperature of (a) 2000 K, (b) 3000 K and (c) 3500 K after 5 ps of the FPMD simulation. Both of the top and side views are displayed.

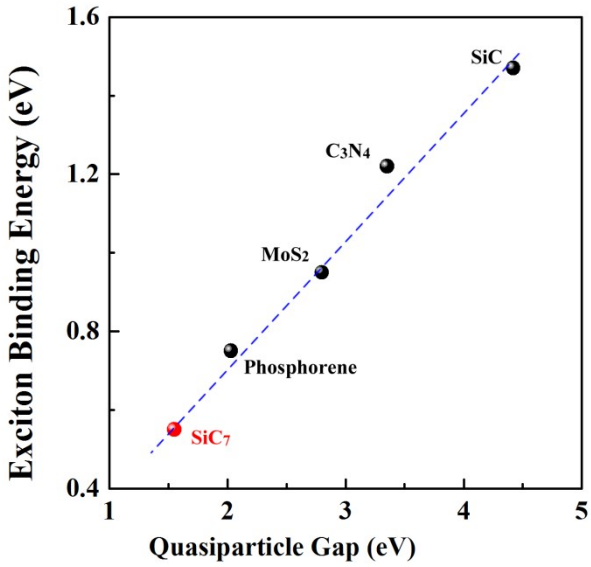

Fig. S3 The exciton binding energy versus the QP band gap for various representative

2D materials. The dashed line represents the fitted linear relation. The exciton binding energies of SiC, C_3N_4, MoS_2 are obtained from ref.[5], ref.[6] and ref.[7], respectively.

Reference

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