Supplementary Information for
“Explore the planar and nonplanar siligraphene: a first-principles study”

We studied two additional Si distributions in 2×2 g-SiC\textsubscript{7} as depicted in Fig. S1. For each Si distribution, planar and nonplanar structures are calculated. It is found that the lattice of planar structure has appreciably larger lattice constants than the corresponding nonplanar one. The Si atoms in the nonplanar structure are buckled in an alternately up and down fashion. The nonplanar structure is considerably more stable than its corresponding planar structure. The nonplanar structures shown in Fig. S1 (a) and (b) are 19.68 and 178.5 meV/atom lower in energy than their planar counterparts. The Si-Si bonds in g-SiC\textsubscript{7} shown in Fig. S1(b) have very high tendency to be buckled. The lattice constants, bondlengths and the height of buckling are listed in Table S1.

Table S1 The lattice parameters, C-C and Si-C bond lengths and buckling h of the optimized g-SiC\textsubscript{7} with Si distributions as shown in Fig. S1. The letters a and b in the first column correspond the structures shown in Fig. S1 (a) and (b), respectively.

<table>
<thead>
<tr>
<th>Structure</th>
<th>a=b(Å)</th>
<th>C-C</th>
<th>Si-C</th>
<th>h(Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>a-g-SiC\textsubscript{7}-flat</td>
<td>10.589</td>
<td>1.466/1.577</td>
<td>1.719</td>
<td>0</td>
</tr>
<tr>
<td>a-g-SiC\textsubscript{7}-buckled</td>
<td>10.348</td>
<td>1.441/1.513</td>
<td>1.757</td>
<td>1.66</td>
</tr>
<tr>
<td>b-g-SiC\textsubscript{7}- flat</td>
<td>10.669</td>
<td>1.416/1.494</td>
<td>1.733</td>
<td>0</td>
</tr>
<tr>
<td>b-g-SiC\textsubscript{7}-buckled</td>
<td>10.209</td>
<td>1.443/1.495</td>
<td>1.919</td>
<td>2.24</td>
</tr>
</tbody>
</table>