

## Support Information:

### Two-Dimensional g-CN<sub>2</sub>/GeC Heterojunctions: Desirable Visible-Light Photocatalyst and Optoelectronic Device

Ying Zhang<sup>a</sup>, Liang Xu<sup>a,b,c,\*</sup>, Hang Liu<sup>a</sup>, Bo Zhang<sup>a</sup>, Ling-Ling Wang<sup>c</sup>

<sup>a</sup> Energy Materials Computing Center, School of Energy and Mechanical Engineering, Jiangxi University of  
Science and Technology, Nanchang, 330013, China

<sup>b</sup> Faculty of Materials Metallurgy and Chemistry, Jiangxi University of Science and Technology, Ganzhou, 341000,  
China

<sup>c</sup> Key Laboratory for Micro-Nano Optoelectronic Devices of Ministry of Education, School of Physics and  
Electronics, Hunan University, Changsha, 410082, China

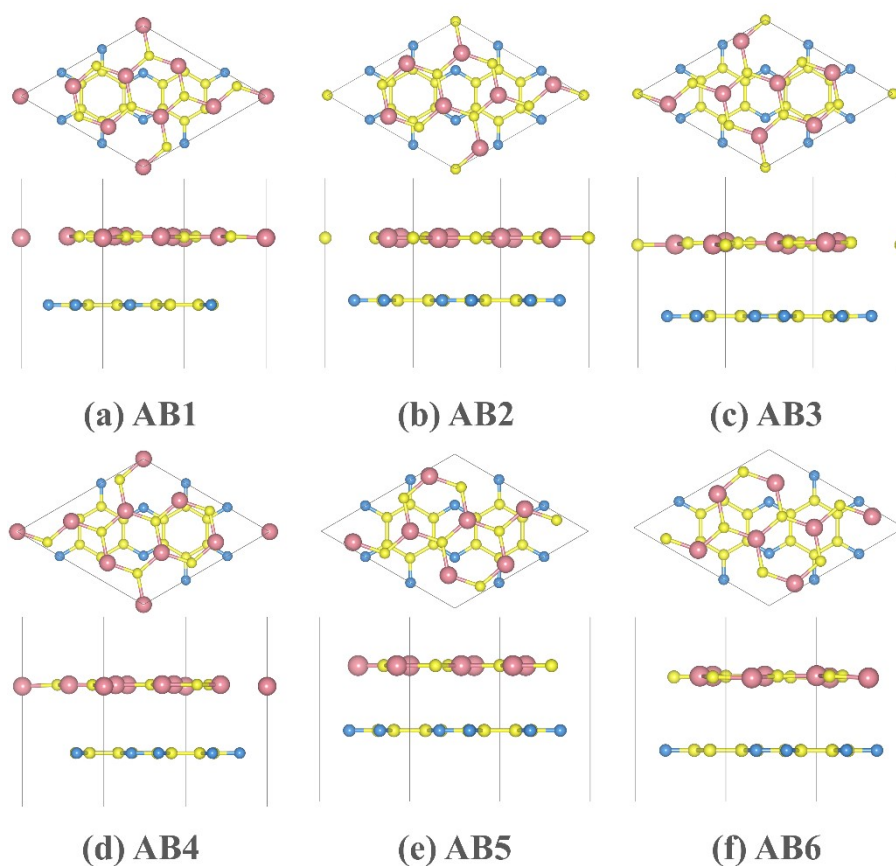


Fig. S1 The top views (top) and side views (bottom) of the six different stacked C<sub>2</sub>N/GeC heterojunctions with (a) AB1 stacking, (b) AB2 stacking, (c) AB3 stacking, (d) AB4 stacking, (e) AB5 stacking, and (f) AB6 stacking, which are drawn by Visualization for Electronic and Structural Analysis (VESTA) software package.

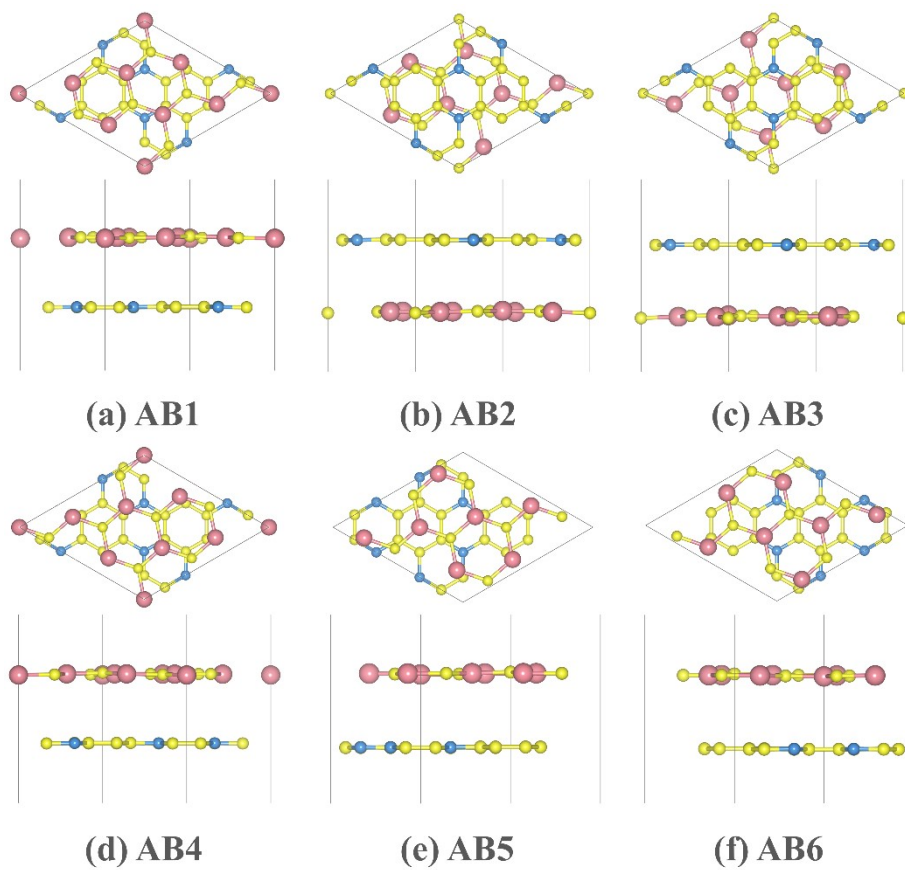


Fig. S2 The top views (top) and side views (bottom) of the six different stacked C<sub>3</sub>N/GeC heterojunctions with (a) AB1 stacking, (b) AB2 stacking, (c) AB3 stacking, (d) AB4 stacking, (e) AB5 stacking, and (f) AB6 stacking, which are drawn by Visualization for Electronic and Structural Analysis (VESTA) software package.

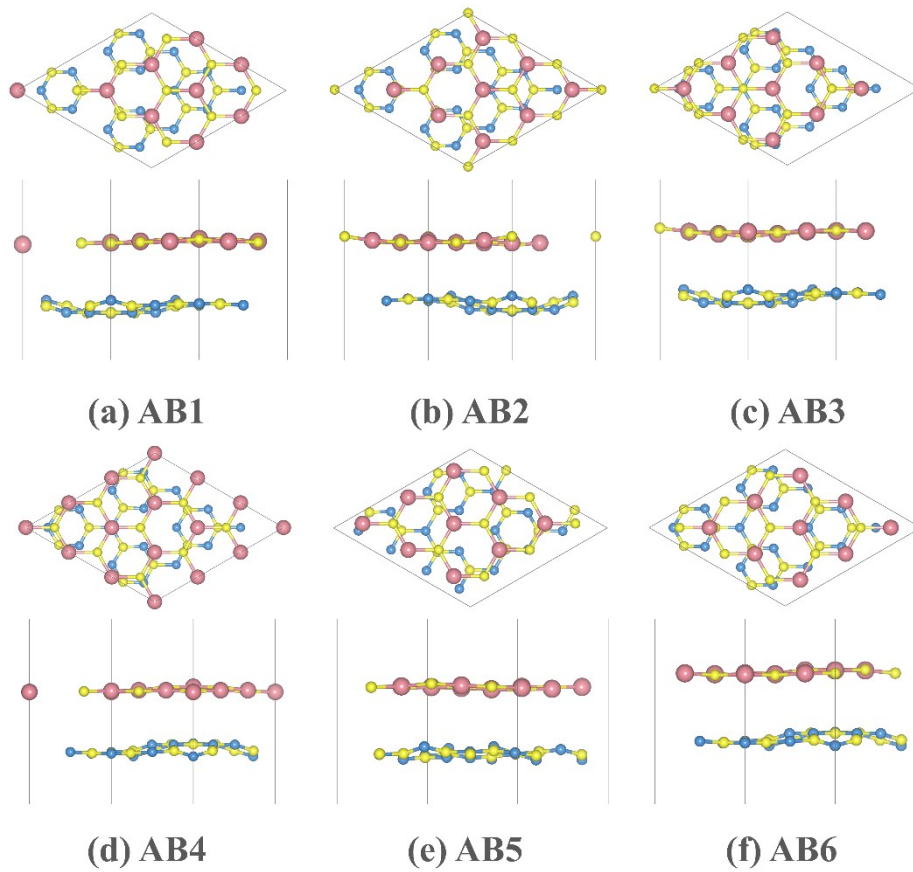


Fig. S2 The top views (top) and side views (bottom) of the six different stacked g-C<sub>3</sub>N<sub>4</sub>/GeC heterojunctions with (a) AB1 stacking, (b) AB2 stacking, (c) AB3 stacking, (d) AB4 stacking, (e) AB5 stacking, and (f) AB6 stacking, which are drawn by Visualization for Electronic and Structural Analysis (VESTA) software package.

**Table S1** The optimized-geometry interlayer distance  $d$  (Å), interlayer binding energy  $E_b$  (eV/atom) of  $C_2N/GeC$ ,  $C_3N/GeC$  and  $g-C_3N_4/GeC$  heterojunctions.

$C_2N/GeC$	<i>AB1</i>	<i>AB2</i>	<i>AB3</i>	<i>AB4</i>	<i>AB5</i>	<i>AB6</i>
$d$ (Å)	3.472	3.492	3.487	3.469	3.498	3.497
$E_b$ (eV)	-0.360	-0.365	-0.364	-0.360	-0.361	-0.368
$C_3N/GeC$	<i>AB1</i>	<i>AB2</i>	<i>AB3</i>	<i>AB4</i>	<i>AB5</i>	<i>AB6</i>
$d$ (Å)	3.478	3.481	3.492	3.480	3.481	3.485
$E_b$ (eV)	-0.780	-0.780	-0.780	-0.781	-0.803	-0.800
$g-C_3N_4/GeC$	<i>AB1</i>	<i>AB2</i>	<i>AB3</i>	<i>AB4</i>	<i>AB5</i>	<i>AB6</i>
$d$ (Å)	3.264	3.235	3.187	3.327	3.185	3.254
$E_b$ (eV)	-3.082	-3.357	-3.140	-3.170	-3.288	-3.086