Supporting information

Evaluation procedure of photocatalysts for VOCs degradation from the view of density functional theory calculations: g-C_3N_4 dots/graphene as an example

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Text S1 The bandgaps of 5×5×1 and 10×10×1 g-C_3N_4 dots/graphene are both 0.009 eV from our calculation with GGA-PBE as shown in Fig. S4(a), while the corresponding adsorption spectrum is also consistent with each other as shown in Fig. S4(b). Therefore, the influence of size effect of the supercell is insignificant.

Text S2 There is big difference for the efficiency of formaldehyde degradation with or without the presence of ·OH radical or both ·OH and $\cdot O_2^-$ radicals. In addition, the reaction rate of formaldehyde degradation under both ·OH and $\cdot O_2^-$ radicals is quicker than that with ·OH radical only because of the shorter reaction pathways as shown in Fig. S7. Noted $\cdot O_2^-$ only plays an insignificant effect on the degradation of formaldehyde.

Table S1 The total and interface interaction energies of the four stacking configurations

Structure	Figure 1a	Figure 1b	Figure 1c	Figure 1d
E_{total}/eV	-9941.846	-9941.833	-11489.229	-11489.415
E_{ads}/eV	-0.462	-0.449	-19.540	-19.727

Table S2 Different configurations of VOCs adsorption

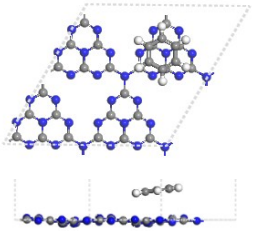
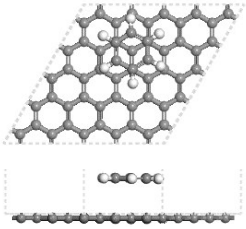
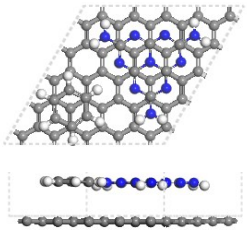
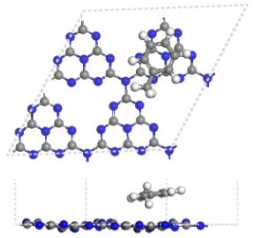
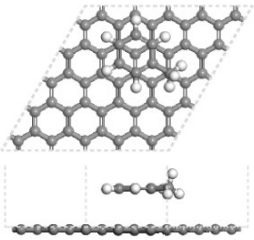
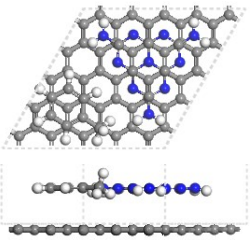
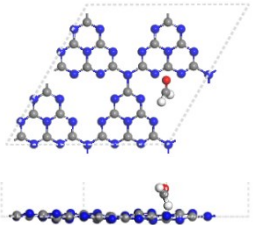
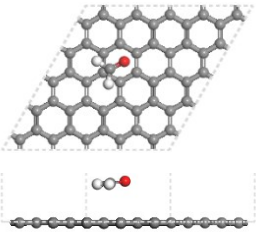
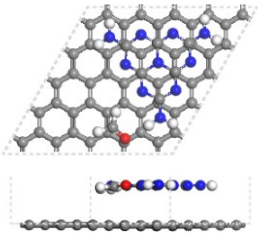
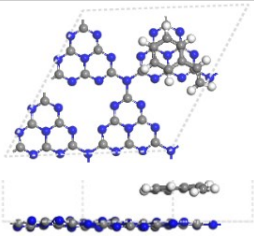
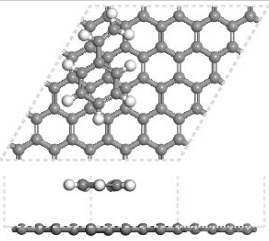
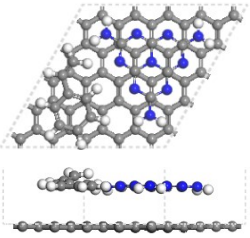
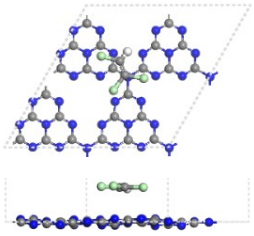
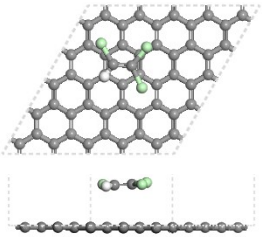
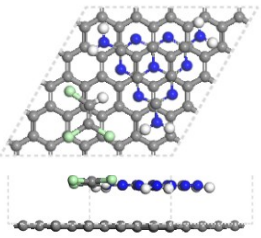
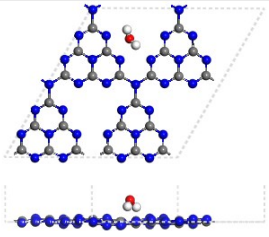
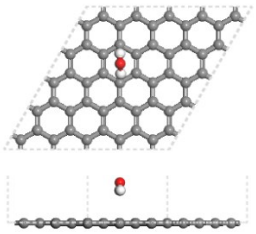
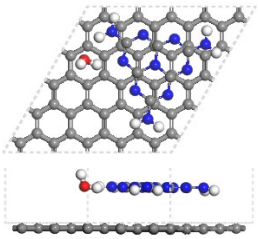
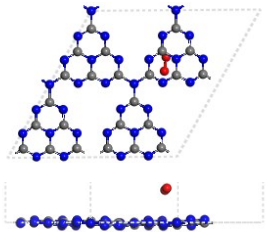
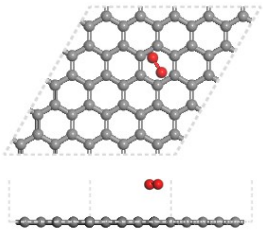
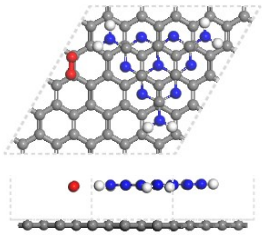
	$g\text{-}C_3N_4$	graphene	complex
Benzene			
Toluene			
Formaldehyde			
Styrene			
TCE			

Table S3 Different configurations of H_2O and O_2 adsorption

	g-C_3N_4	graphene	complex
H_2O			
O_2			

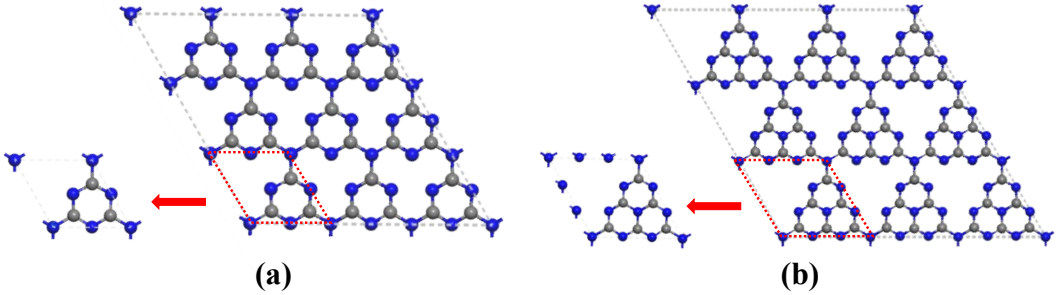


Fig. S1 The scheme of *s-triazine* g-C_3N_4 (a) and *tri-s-triazine* g-C_3N_4 (b). Atom color code in this and following figures: carbon (grey), nitrogen (blue), hydrogen (white).

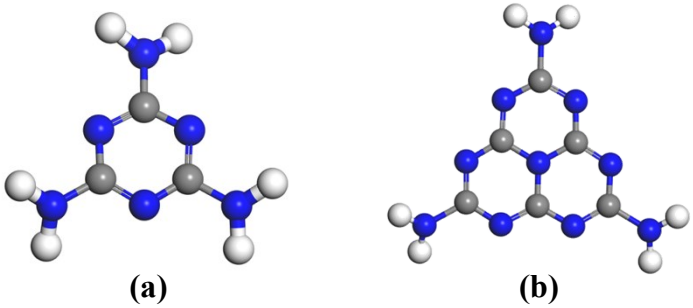


Fig. S2 The scheme of *s-triazine* g-C_3N_4 dots (a) and *tri-s-triazine* g-C_3N_4 dots (b).

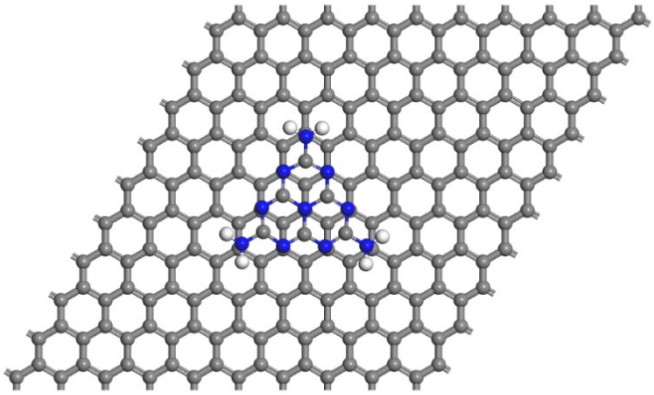


Fig. S3 The configuration of g-C_3N_4 dots in graphene with 10×10×1 supercell. The adsorption energy is -19.699 eV.

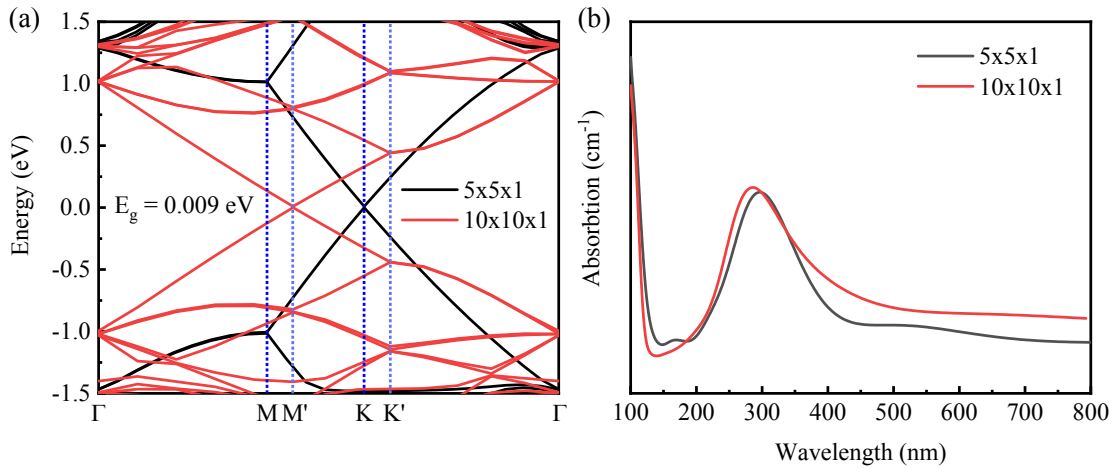
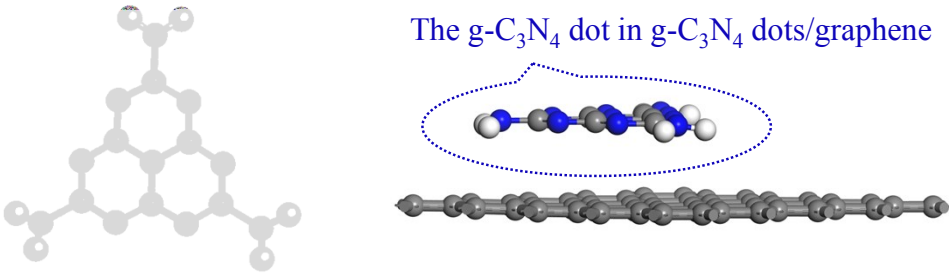


Fig. S4 The band structure (a) and optical adsorption (b) of g-C_3N_4 dots in 5×5×1 and 10×10×1 graphene.



(a) pristine g-C_3N_4 dot (p-CND) **(b) adsorbed g-C_3N_4 dot (a-CND)**

Fig. S5 The *tri-s-triazine* g-C_3N_4 dots under pristine condition (a) and composite condition (b).

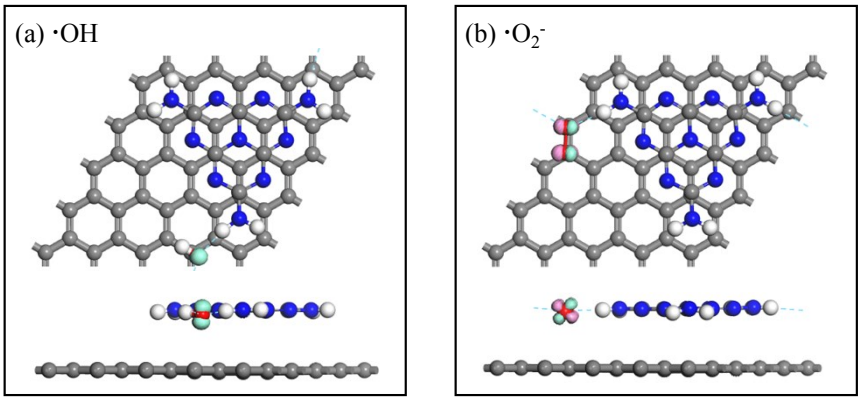


Fig. S6 The spin density of ·OH (a) and $\cdot O_2^-$ (b) on g-C_3N_4 dots/graphene. The colors of spin density represent the different directions of spin.

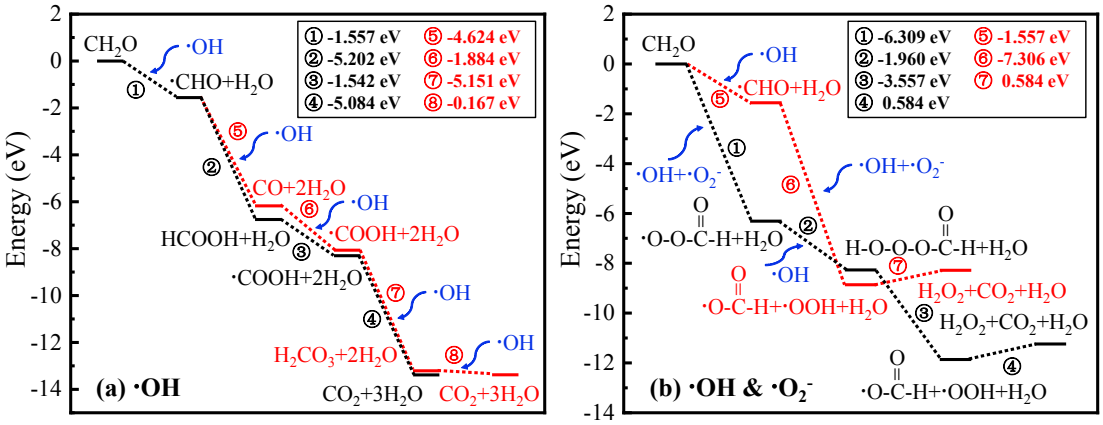


Fig. S7 The reaction pathways for formaldehyde degradation in the presence of ·OH radical (a) and both ·OH and $\cdot O_2^-$ radicals (b). Red and black lines represent the different reaction pathway. Reactants, products and energy barriers are marked in the corresponding places. The numbers represent different reaction steps.