Supporting Information for

KCl-Mediated Dual Electronic Channels in Layered g-C_3N_4 for Enhanced Visible Light Photocatalytic NO Removal

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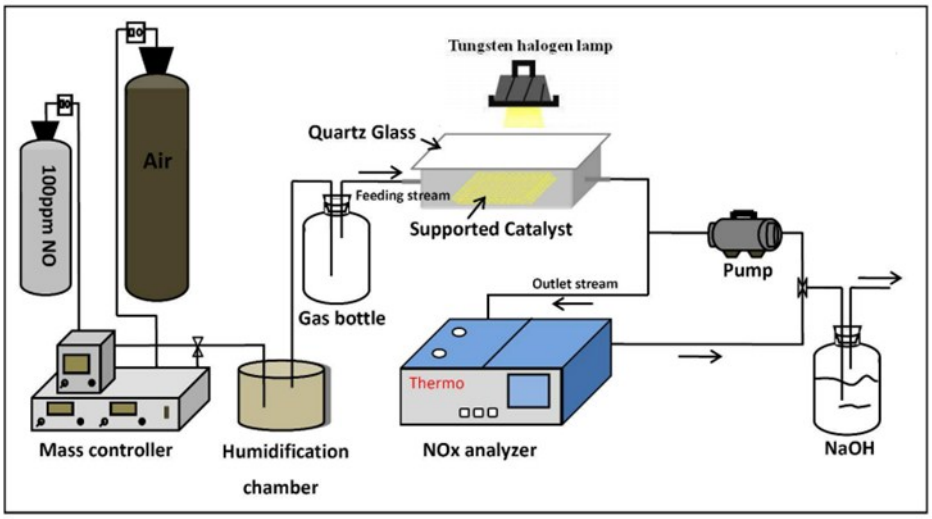

Fig. S1. Schematic of the experimental set-up.

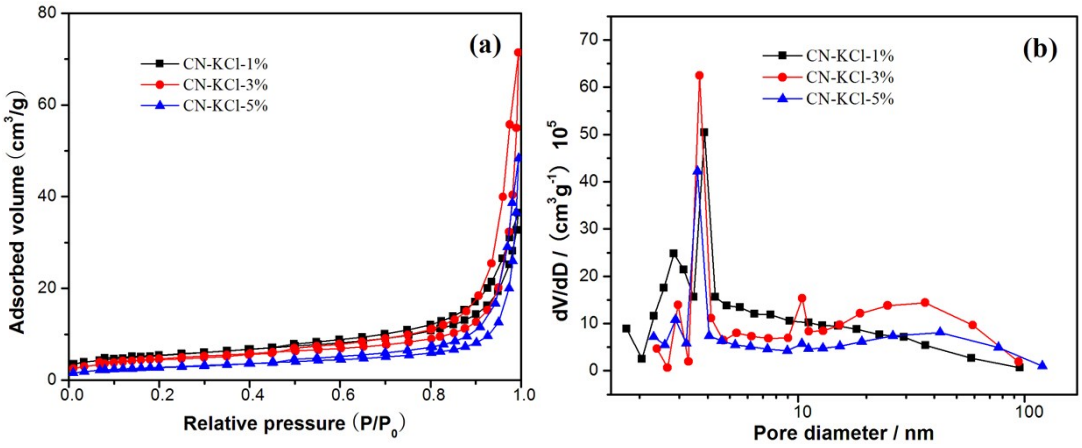

Fig. S2 Nitrogen adsorption-desorption isotherm (a) and pore size distribution (b) of KCl doped g-C_3N_4.

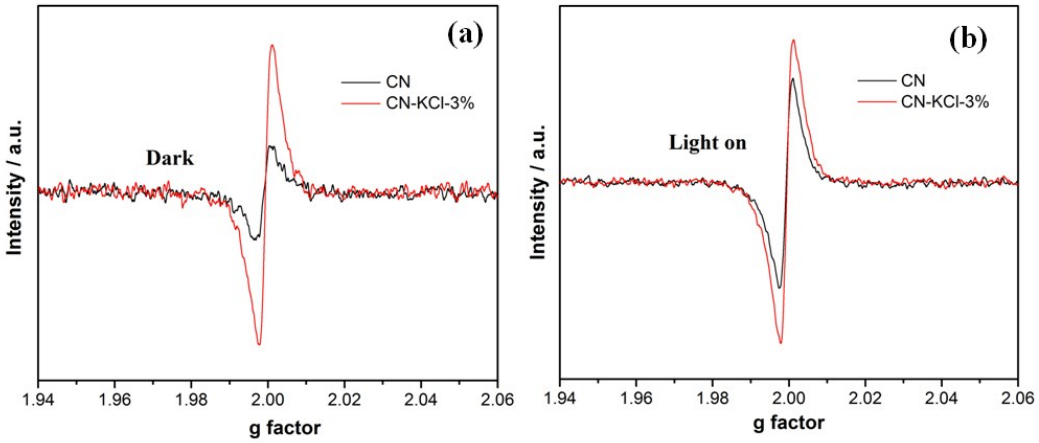

Fig. S3 The electron paramagnetic resonance (EPR) measurements of CN and CN-KCl-3% in the dark (a) and under light irradiation (b).

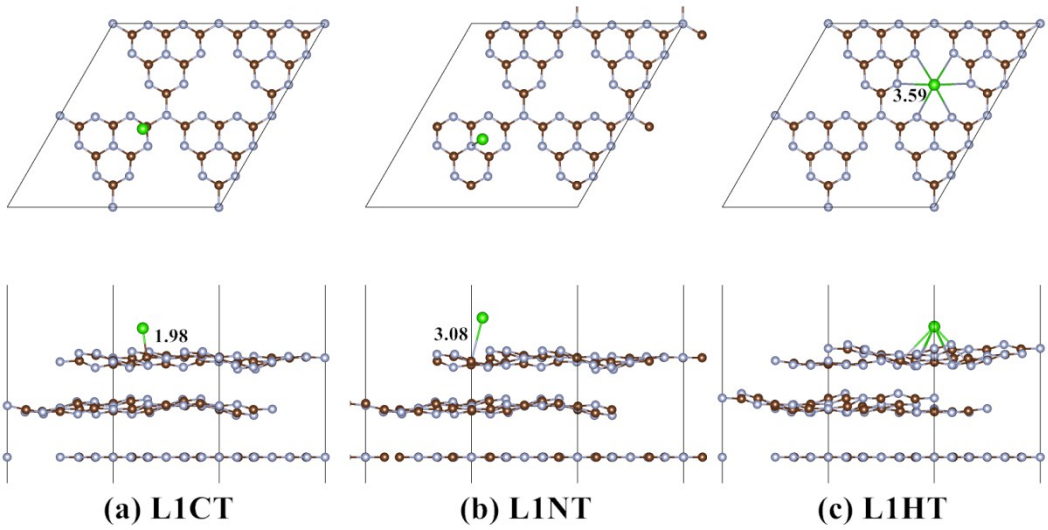

Fig. S4 Adsorption configurations of single Cl atom on the top layer of g-C_3N_4 surface. L1CT denotes that Cl is adsorbed on the top of C atom of the first layer. L1HT denotes that Cl is adsorbed on the top of the cave of the first layer. L1NT denotes that Cl is adsorbed on the top of N atom of the first layer. In the upper plane (top view), the two layers in the bottom was removed for clarity.

Table S1. Calculated total energy of relaxed supercell model.

Sites	L1CT	L1HT	L1NT	L2HT	L2CT
sole Cl ads.	-2.49	-1.91	-2.44	-0.78	-1.77
KCl ads.	-2.22	-1.32	-1.88	-2.57	
K_Cl inter.	0.28	0.59	0.55	-1.79	

Sole Cl ads. is the adsorption of single Cl atom by g-C_3N_4.
KCl ads. is the adsorption of single Cl atom by K pre-adsorbed g-C_3N_4.
Unit is eV.

As shown in Fig. S4 and Table S1, Cl atom is inclined to be adsorbed on the top of C atom, with the lowest adsorption energy of -2.49 eV.

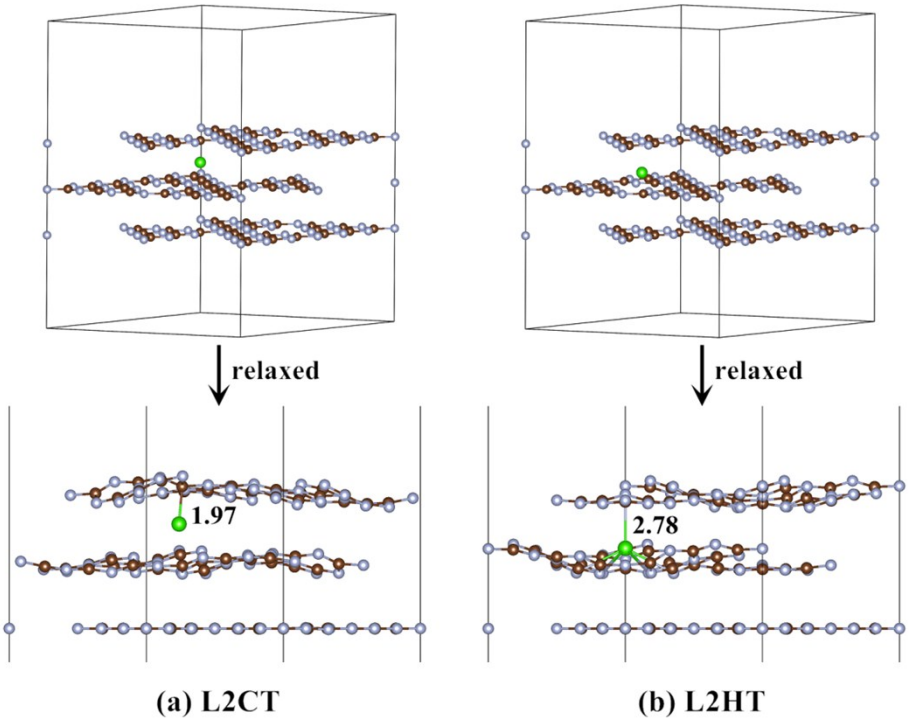

Fig. S5 Adsorption configurations of single Cl atom inserted between the first and the second layer of g-C_3N_4. L2HT denotes that Cl is adsorbed on the top of the cave of the second layer. L2CT denotes that Cl is adsorbed on the top of C atom of the second layer.

As shown in Fig. S5 and Table S1, Cl atom is inclined to be adsorbed on the C atom of the second layer, with a much lower adsorption energy -1.77 eV.

According to the results demonstrated in Fig. S4, Fig. S5 and Table S1, Sole Cl atom is inclined to be adsorbed on the surface C atom of g-C_3N_4.

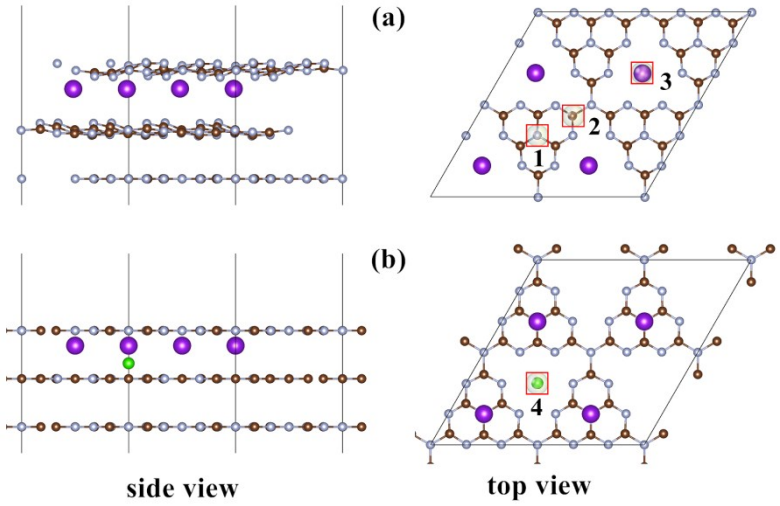

Fig. S6 Four different adsorption sites for Cl atom in K pre-intercalated g-C_3N_4. The sites 1~3 exist on the surface of g-C_3N_4, which are denoted as L1NT, L1CT and L1HT, respectively. The site 4 exists on the top of the cave of the second layer of g-C_3N_4 and are denoted as L2HT.

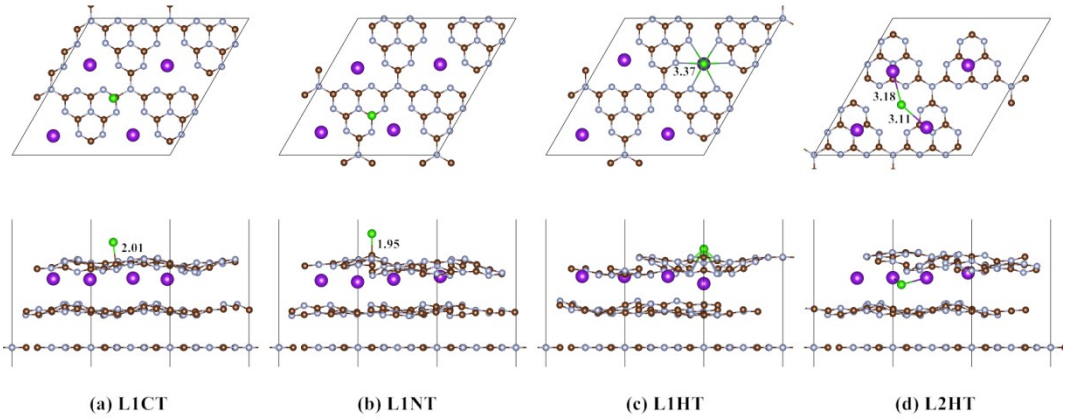

Fig. S7 Four relaxed configurations of Cl atom adsorbed in K pre-intercalated g-C_3N_4 (top view and side view).

According to the results demonstrated in Fig. S7 and Table S1, when K is pre-intercalated into g-C_3N_4, Cl atom is inclined to be adsorbed on the top of the cave in the interlayer. Namely, the existence of K atoms decreases the surface adsorption of Cl atoms and enhances the adsorption of Cl atom in the interlayer because of the interaction between K and Cl atoms.