

Supporting Information

Nitrogen-doped carbon supports with terminated hydrogen and their effects on active gold species: A density functional study

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Color index: bond length (\AA), red

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Table S1. Charge distribution of Au dimer on different supports

Table S2. Mulliken charge of HCl adsorbed on $\text{Au}_2\text{Cl}_6/\text{supports}$

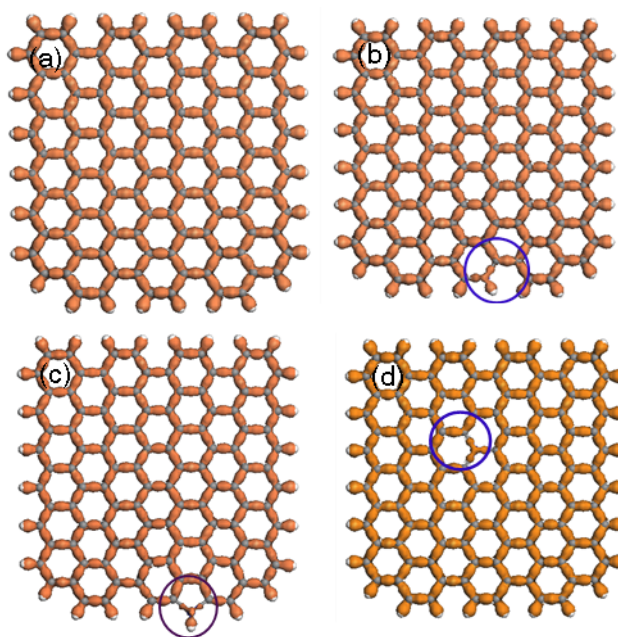


Figure S1. The deformation electron density of different support of (a)GR, (b) GRN-I,

(c) GRN-II and (d) GRN-III. The purple circles show the N-doped site.

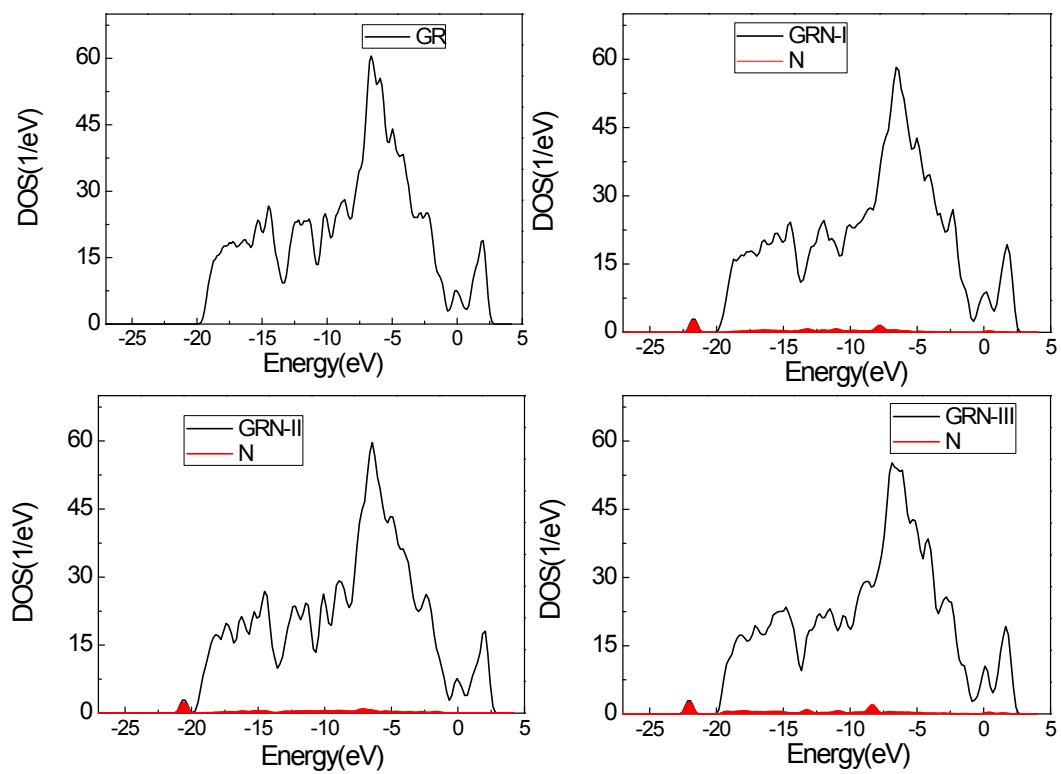


Figure S2. DOS of four supports (a) GR (b) GRN-I (c) GRN-II (d) GRN-III. The red shadow means the contribution of N atom in the total DOS curve.

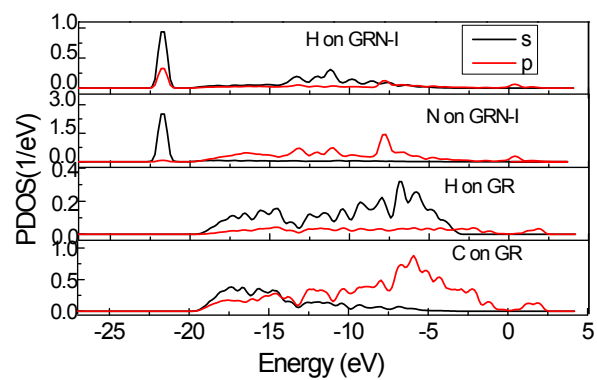


Figure S3. PDOS of H, N atom on N-doped graphene and H, C atom on pristine graphene are arranged from top to bottom

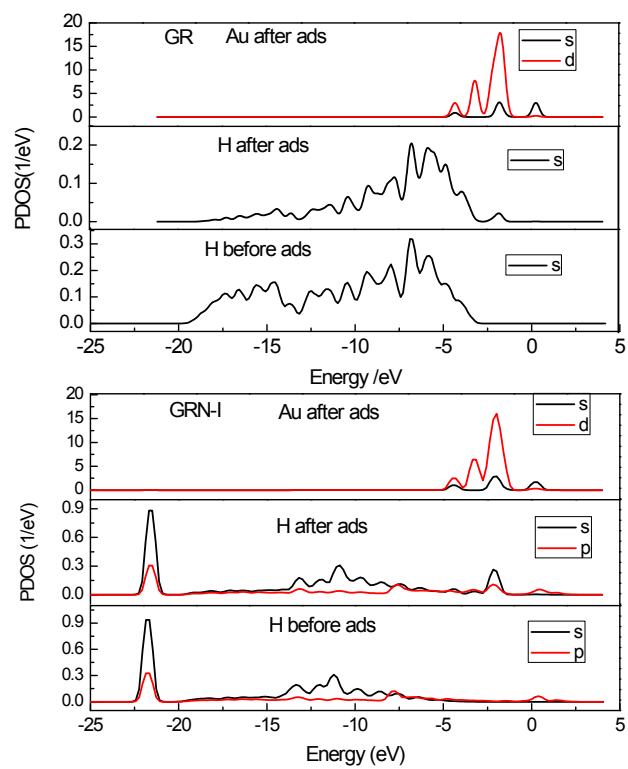


Figure S4. PDOS of Au dimer and H after adsorption for different support (a) GR (b)

GRN-I

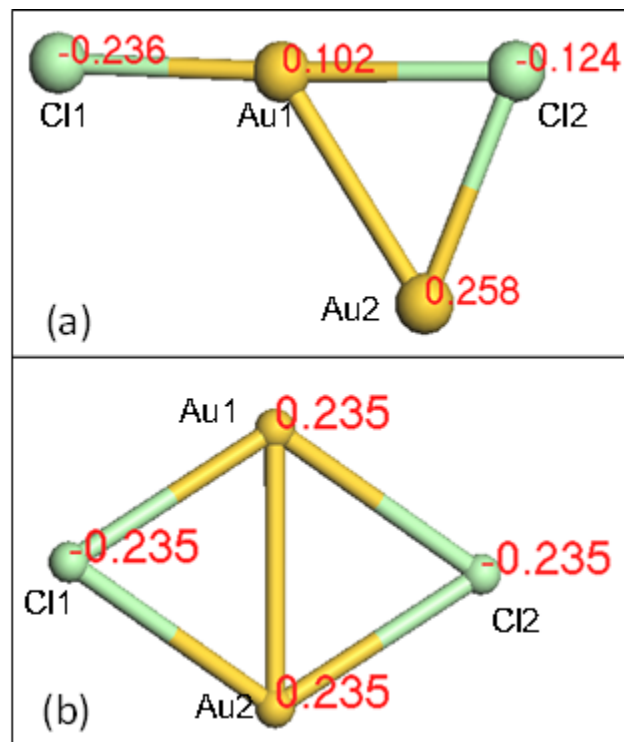


Figure S5. Mulliken charges (red numbers) on the (a) triangular model or (b) tetragonal model. Color index: Au atom-yellow; Cl atom-green.

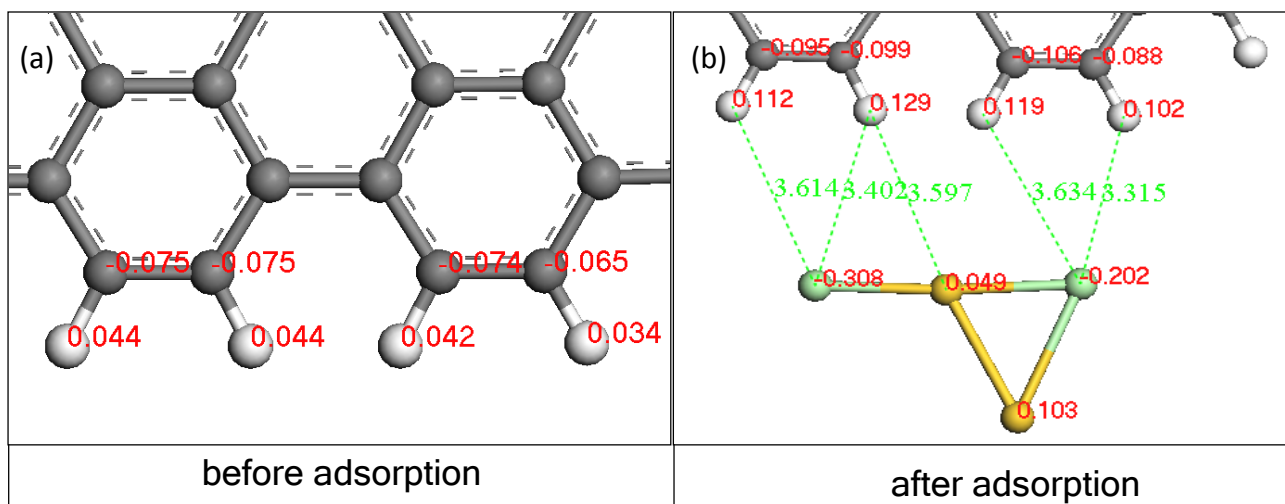


Figure S6. The charge distribution of (a) GR before and after Au_2Cl_2 adsorption (b).

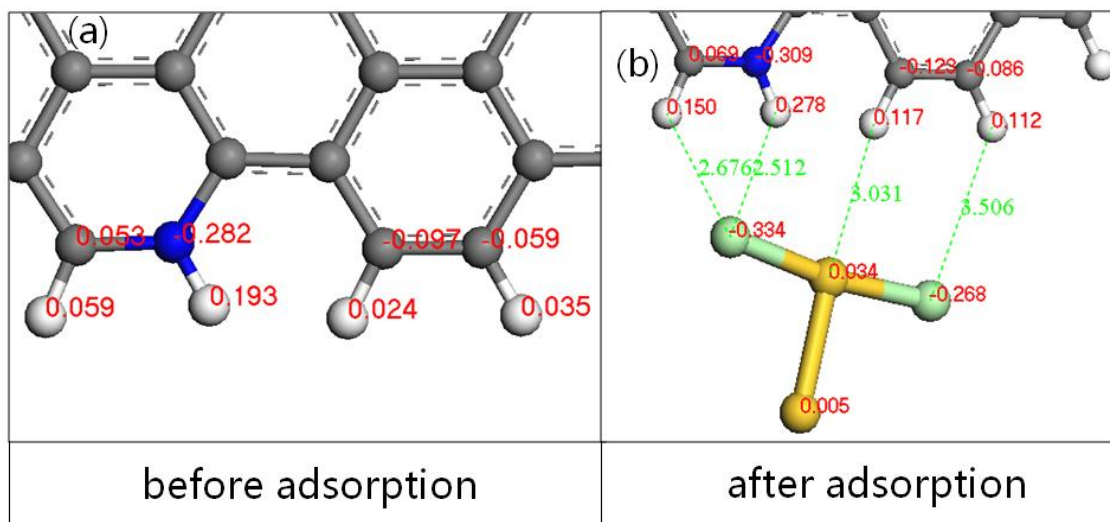


Figure S7. The charge distribution of GRN-I (a) before and after Au_2Cl_2 adsorption

(b).

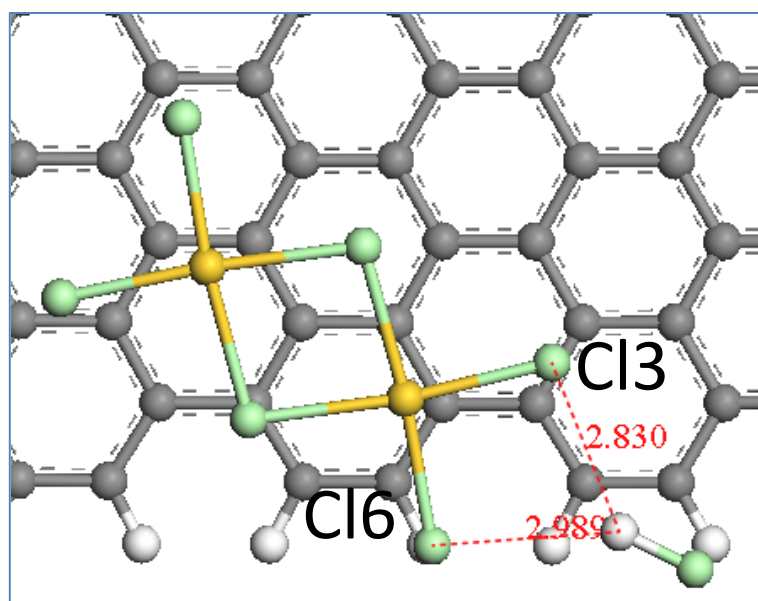


Figure S8. The initial position of HCl on the adsorbed Au₂Cl₆ with the support of GR.

Color index: bond length (Å), red

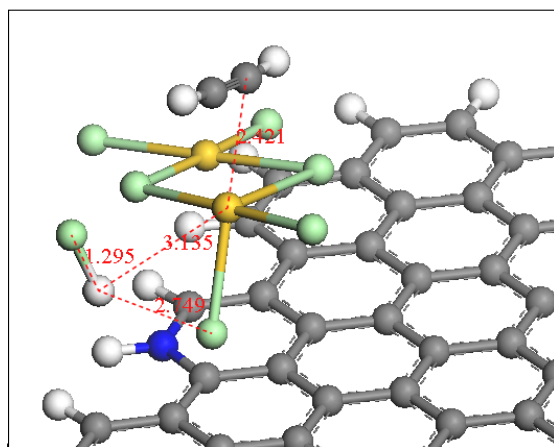


Figure S9. The initial positions of C_2H_2 and HCl on $Au_2Cl_6/GRN-I$.

Table S1. Charge distribution of Au dimer on different supports

Atom number	Au dimer	GR	GRN-I	GRN-II	GRN-III
Au1	0	-0.069	-0.184	-0.110	-0.076
Au2	0	-0.069	-0.149	-0.078	-0.059
Total charge	0	-0.138	-0.333	-0.188	-0.135

Table S2. Mulliken charge of HCl adsorbed on Au₂Cl₆/supports

	Gas phase	GR	GRN-I	GRN-II	GRN-III
H	0.128	0.202	0.197	0.205	0.197
Cl	-0.128	-0.237	-0.246	-0.246	-0.244
Total charge	0	-0.035	-0.049	-0.041	-0.047