Optimizing the Local Charge of Graphene via Iron Doping to Promote the Adsorption of Formaldehyde Molecules—A Density Functional Theory Study

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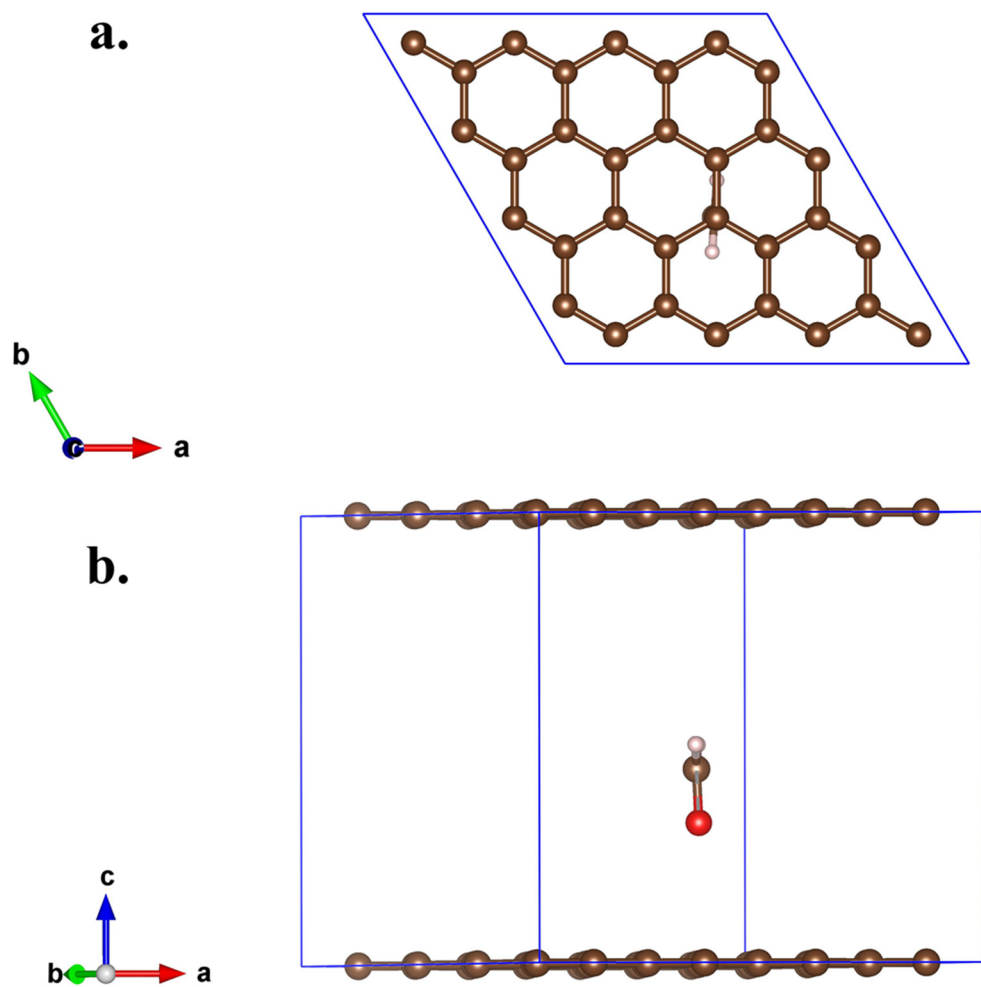* Correspondence: chenc@just.edu.cn; Tel./Fax: +86-0511-85639001

a.

b.

Figure S1. The original configuration (a) of formaldehyde molecules adsorbed on GH substrate.

a.

b.

Figure S2. The original configuration (b) of formaldehyde molecules adsorbed on GH substrate.
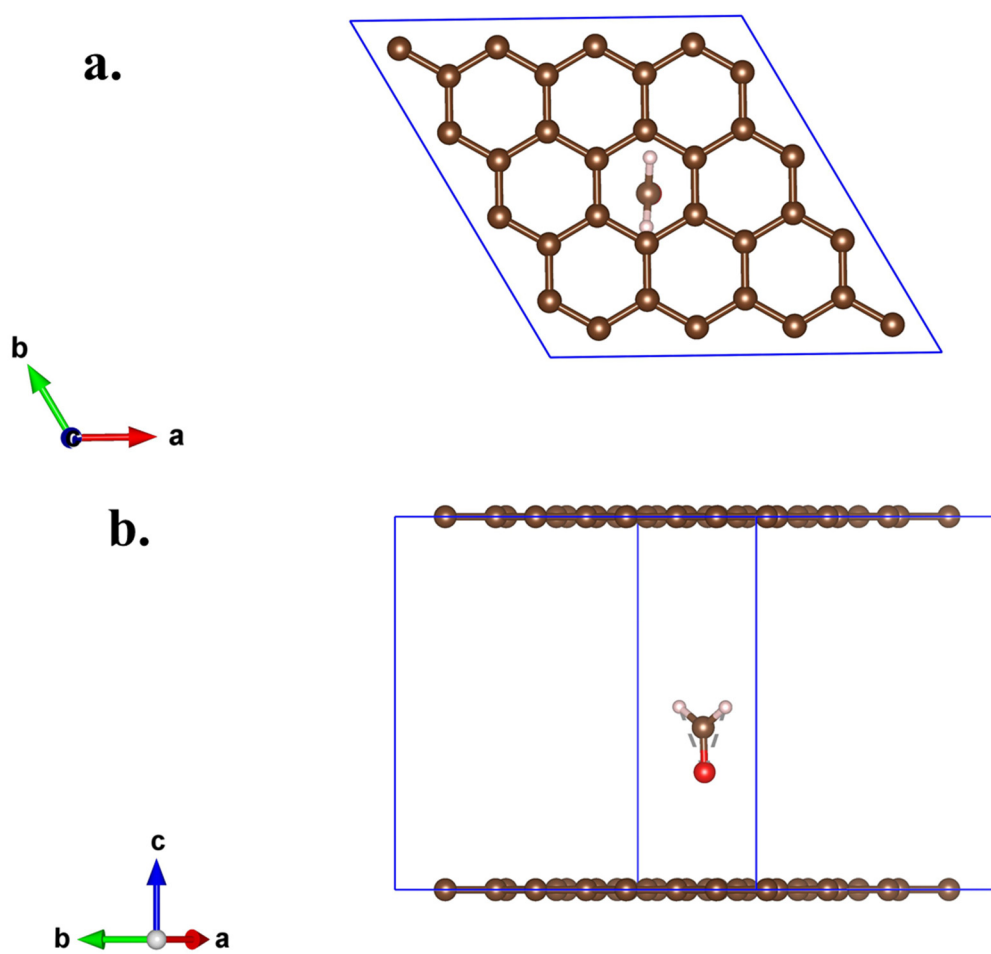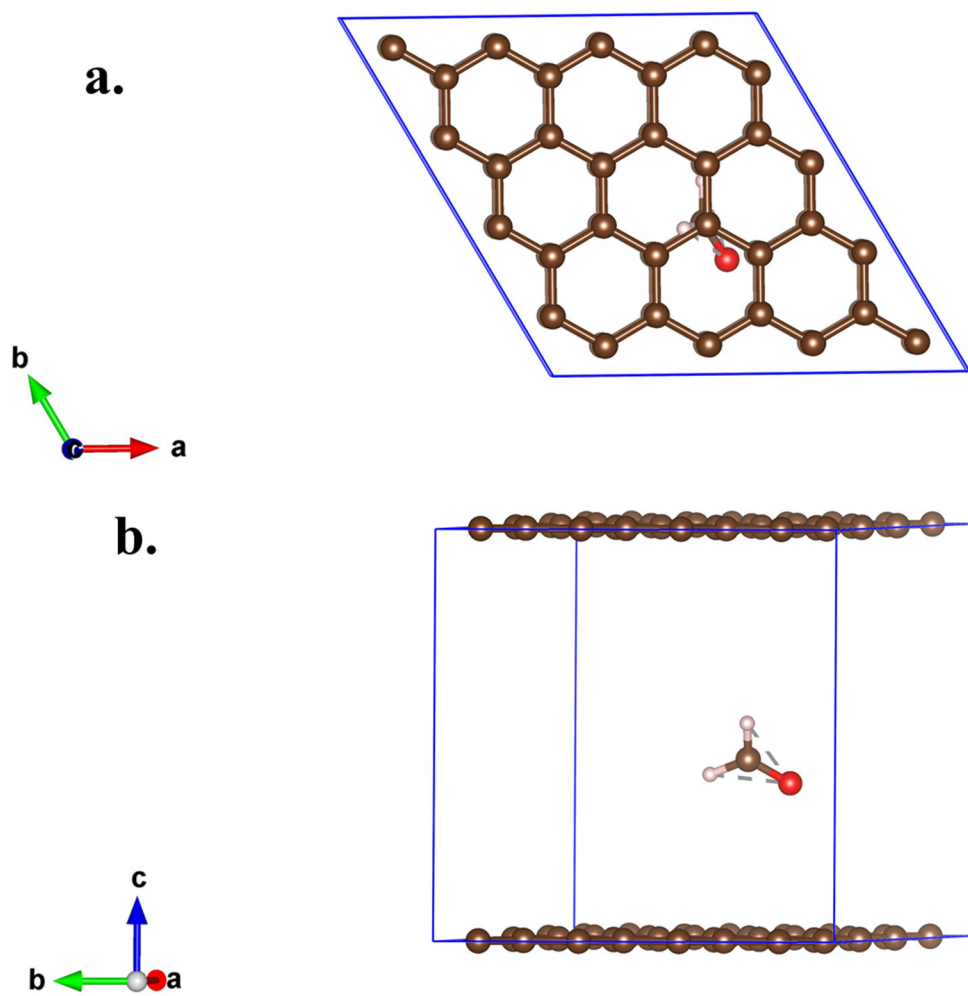
a.

b.

Figure S3. The original configuration (c) of formaldehyde molecules adsorbed on GH substrate.

Figure S4. The original configuration (d) of formaldehyde molecules adsorbed on GH substrate.
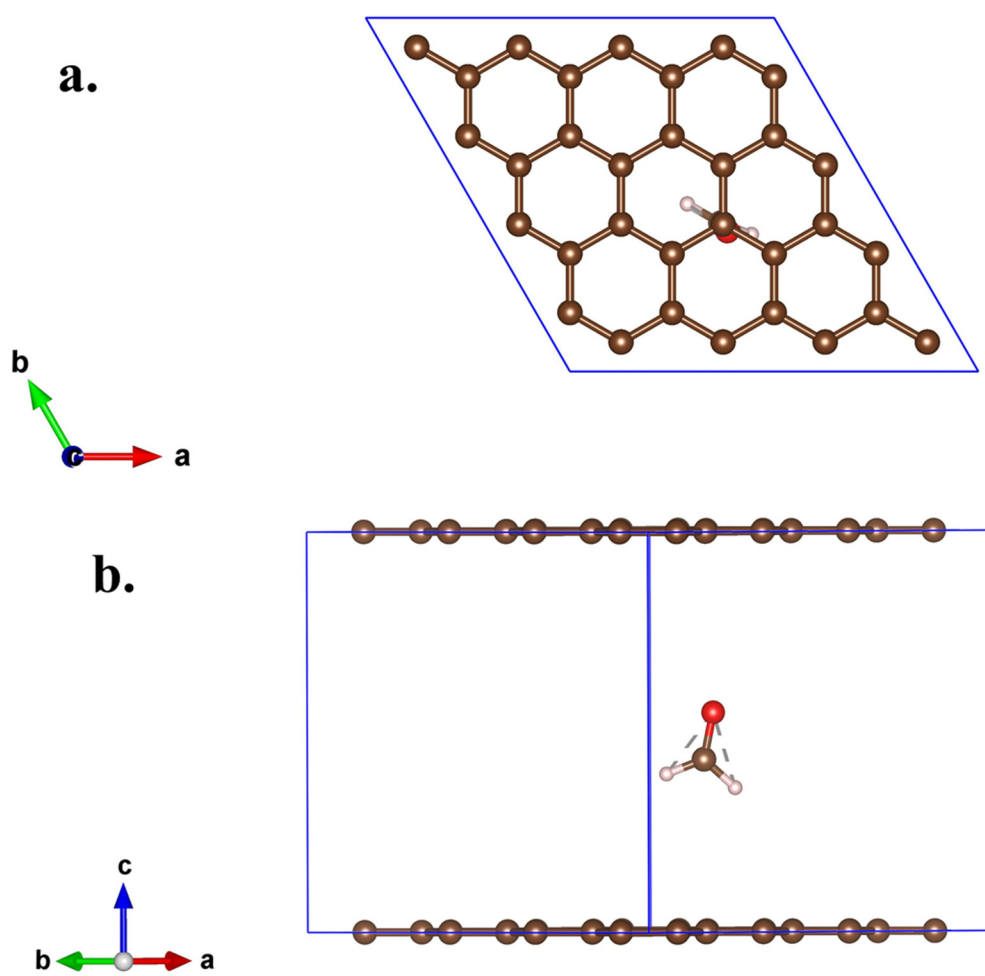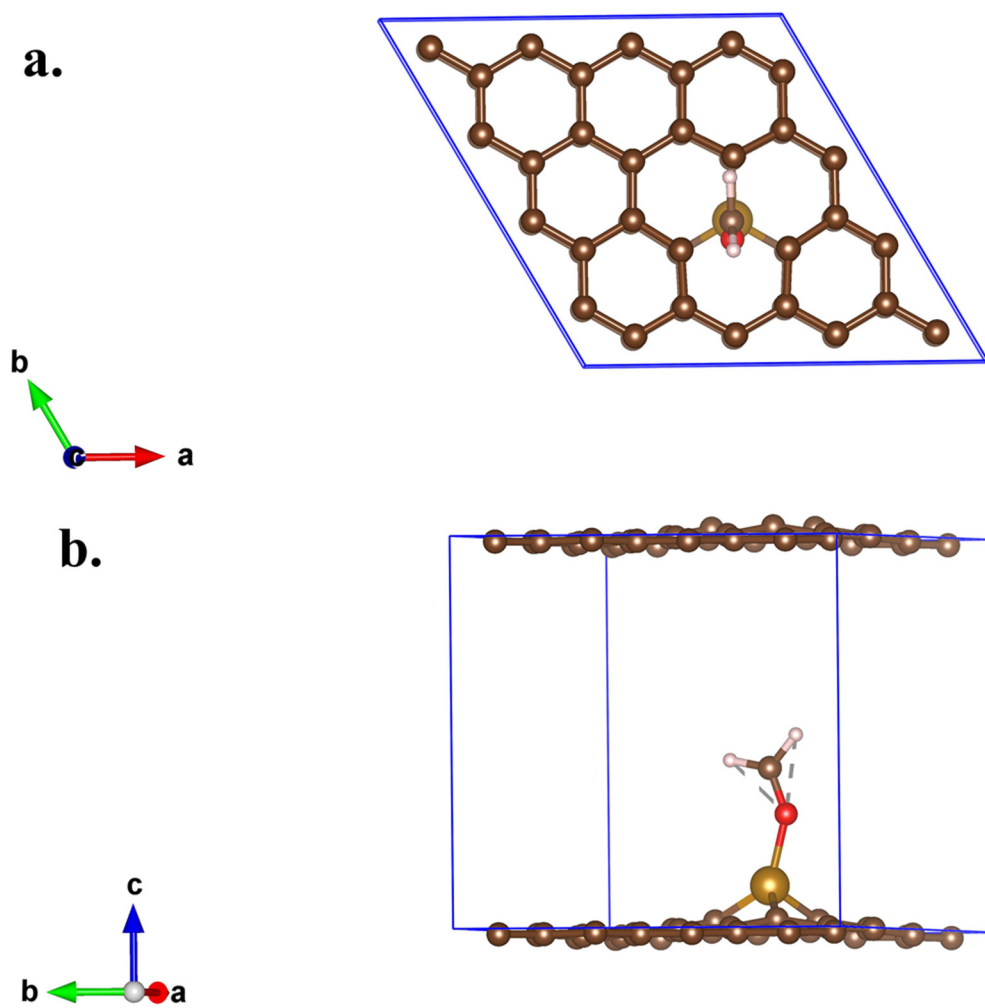
a.

b.

Figure S5. The original configuration (a) of formaldehyde molecules adsorbed on Fe-GH substrate.

Figure S6. The original configuration (b) of formaldehyde molecules adsorbed on Fe-GH substrate.
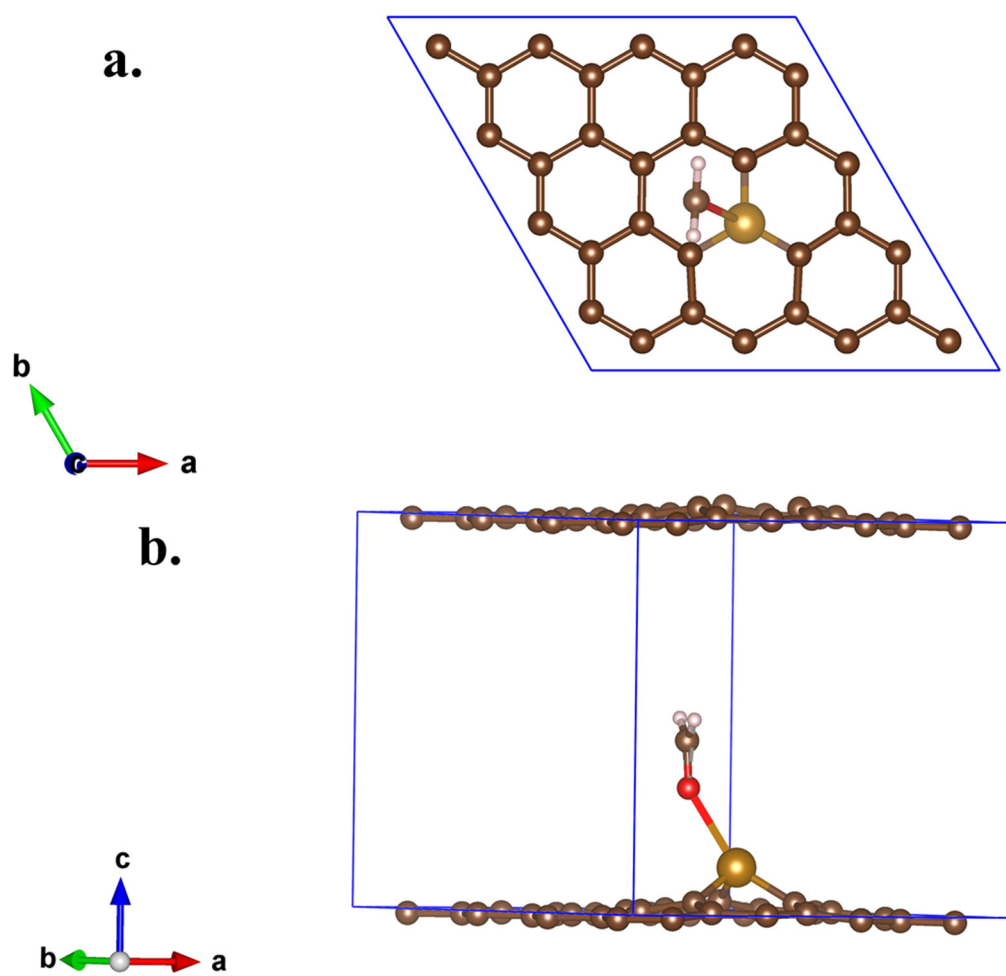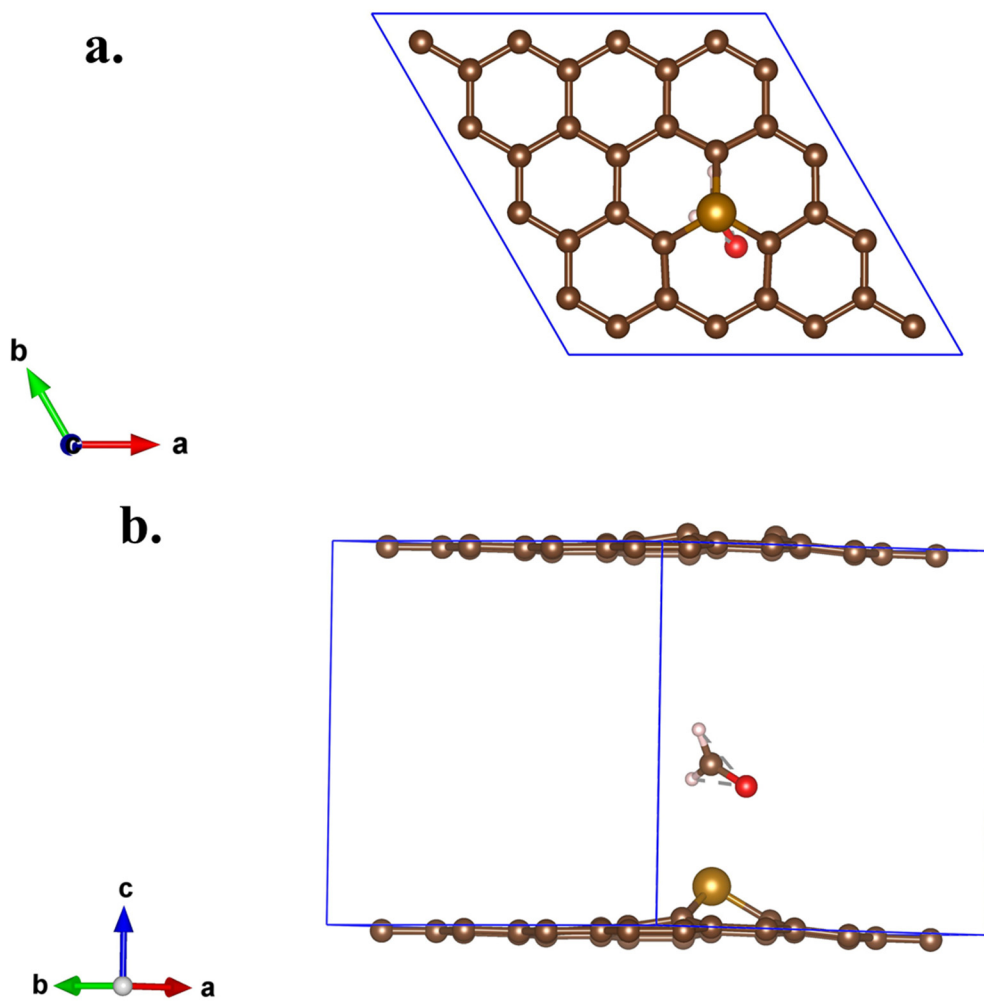
a.

b.

Figure S7. The original configuration (c) of formaldehyde molecules adsorbed on Fe-GH substrate.

a.

b.

Figure S8. The original configuration (d) of formaldehyde molecules adsorbed on Fe-GH substrate.
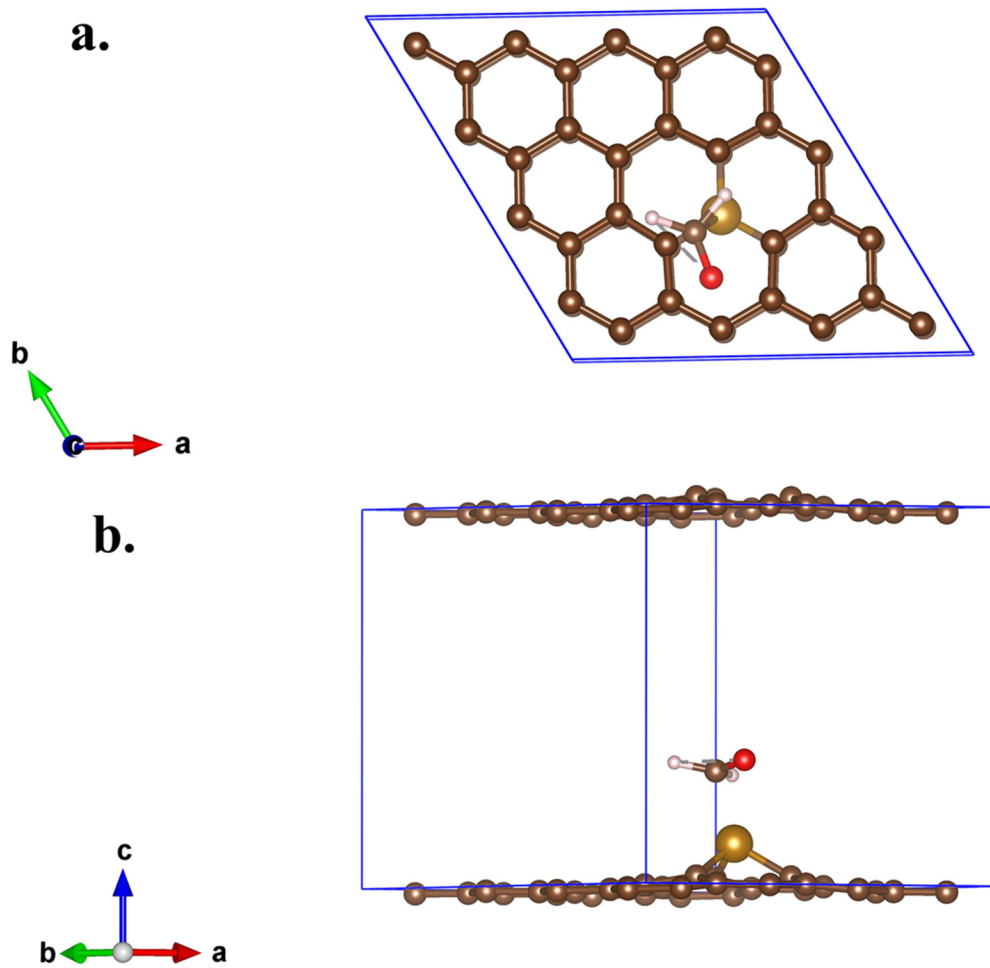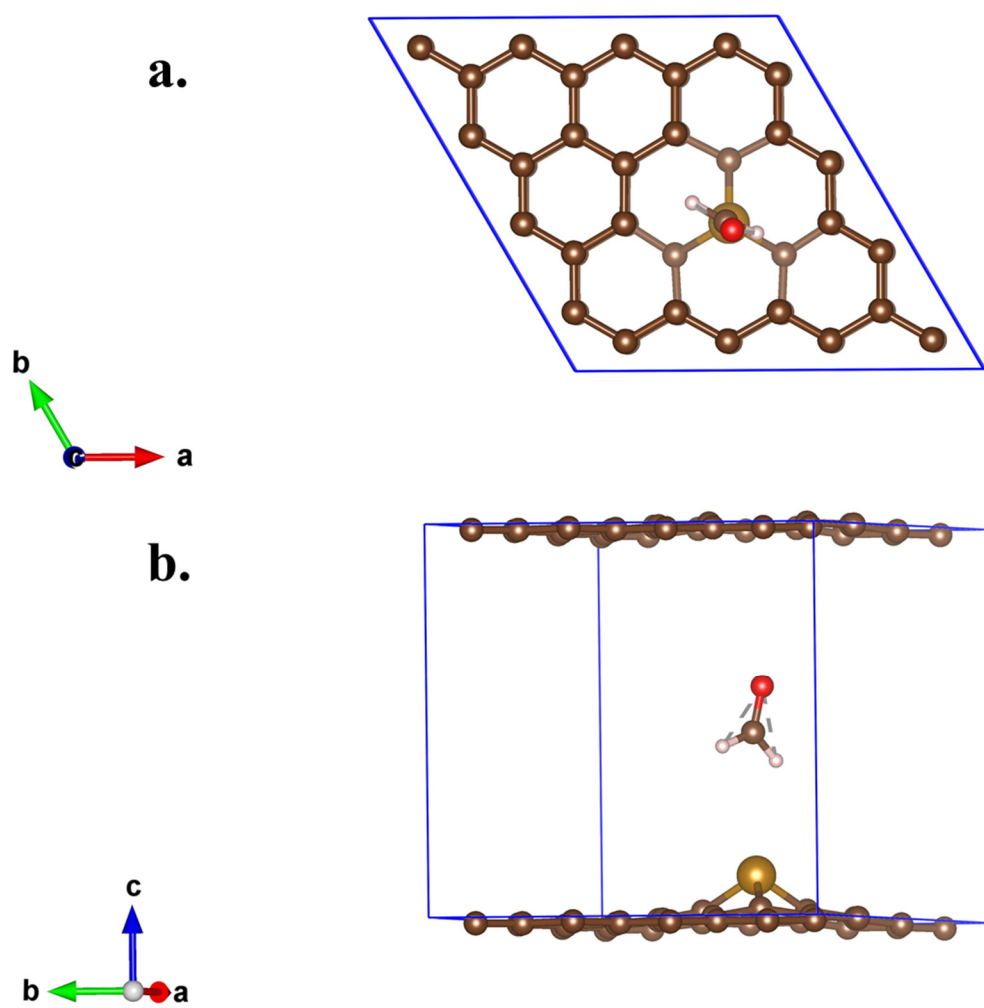
a.

b.

Figure S9. The original configuration (e) of formaldehyde molecules adsorbed on Fe-GH substrate.

Table S1. Bader charge before and after iron doping on GH substrate.

atoms	Before doped	After doped	change
C1	3.962	4.159	0.197
C2	3.971	4.387	0.416
C3	3.987	4.150	0.164
Fe	8.000	7.160	-0.840

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