Electronic Supplementary Material (ESI) for Analyst.

Electronic Supplementary Information (ESI)

Ab initio characterization and experimental validation on the roles of oxygen-containing groups in graphene based formaldehyde sensors

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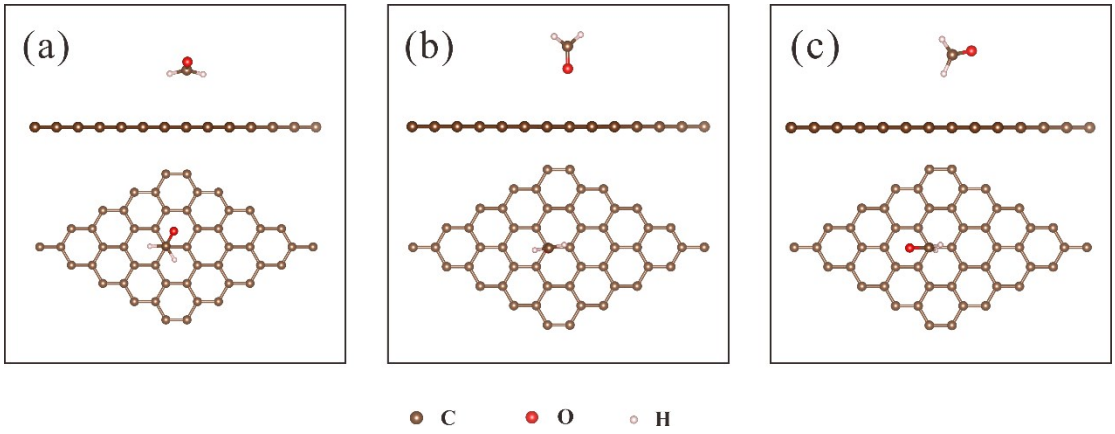

Fig. S1 The optimized structure of HCHO adsorbed on pristine graphene, (a) C-closed; (b) O-closed; (c) H-closed.

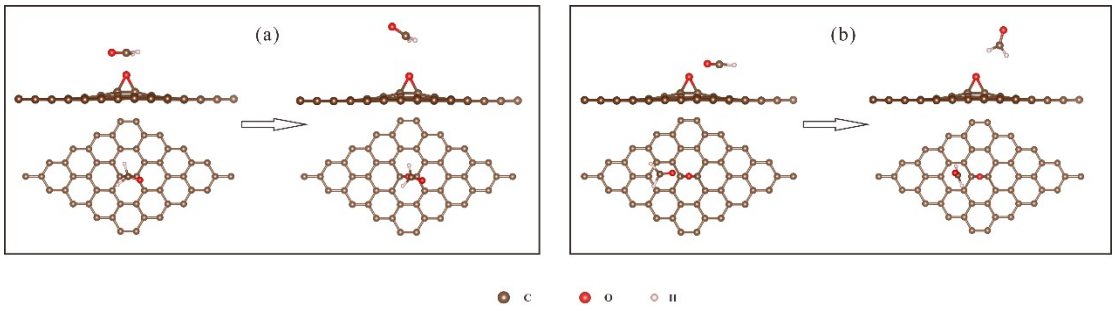

Fig. S2 The adsorption structrue of HCHO on rGO with individual epoxide (rGO-O) for different configurations. The left of the arrow is the initial structure, while the right is the optimized structure.

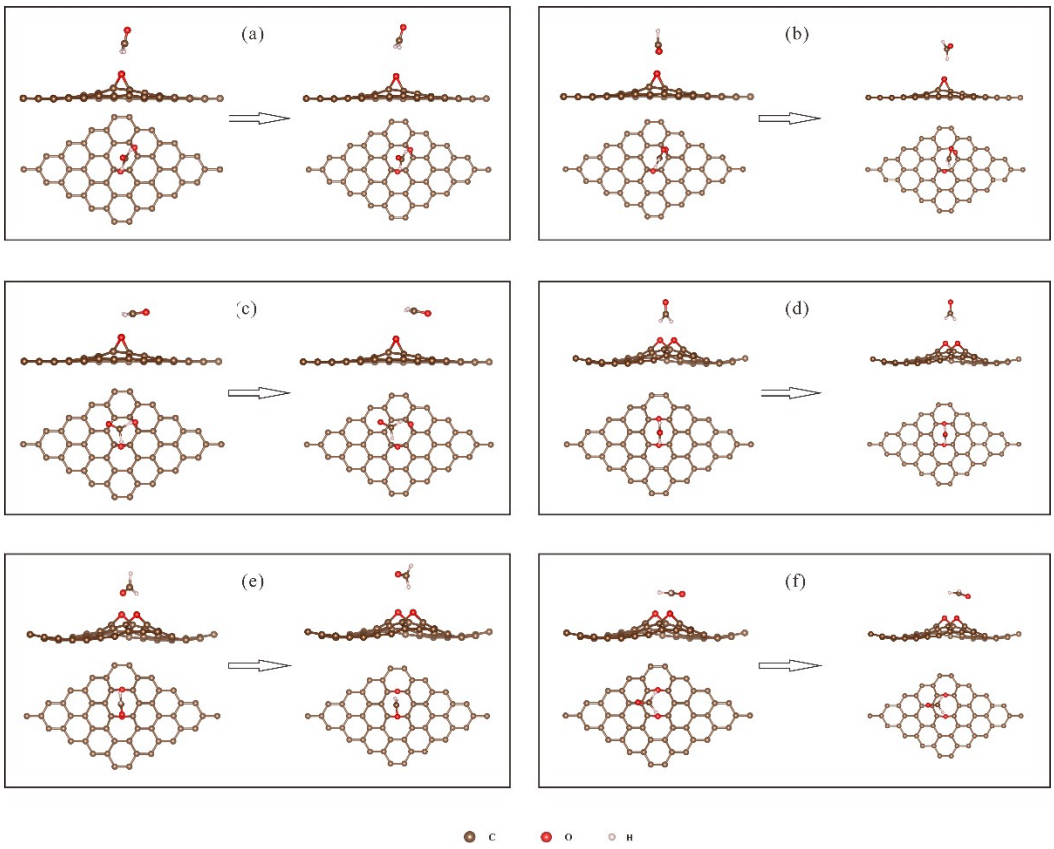

Fig. S3 (a-c) the adsorption structure of HCHO on two epoxides with meta-position (C-O_O-C) with different initial configurations; (e-g) the adsorption of HCHO on two epoxides with para-position (C-O__O-C) with different initial configurations. The left of the arrow is the initial structure, while the right is the optimized structure.

Table S1 The adsorption energy (E_{ads}) and charge transfer (ΔQ) of HCHO molecule adsorbed on rGO with epoxides.

		E_{ads} (meV)	ΔQ *(e)*	atom[a]	orientation[b]
1	'C-O-C'	87	-0.003	C	p
2		81	-0.007	O	d
3		115	-0.006	H&H	u
4	'C-O_O-C'	119	0.025	H&H	u
5		87	0.012	H&O	d
6		85	0.002	H&H	p

7	'C-O__O-C'	87	0.008	H&H	u
8		47	0.006	H&O	d
9		110	0.014	H&H	p

[a] The atom of HCHO molecule close to the oxygen groups, H&H means the two H atom are close to the O atoms of surface. [b] The label u, d, and p mean that the C=O bond of HCHO molecule pointing up (u), down (d), and parallel to the surface (p), starting from C atom.

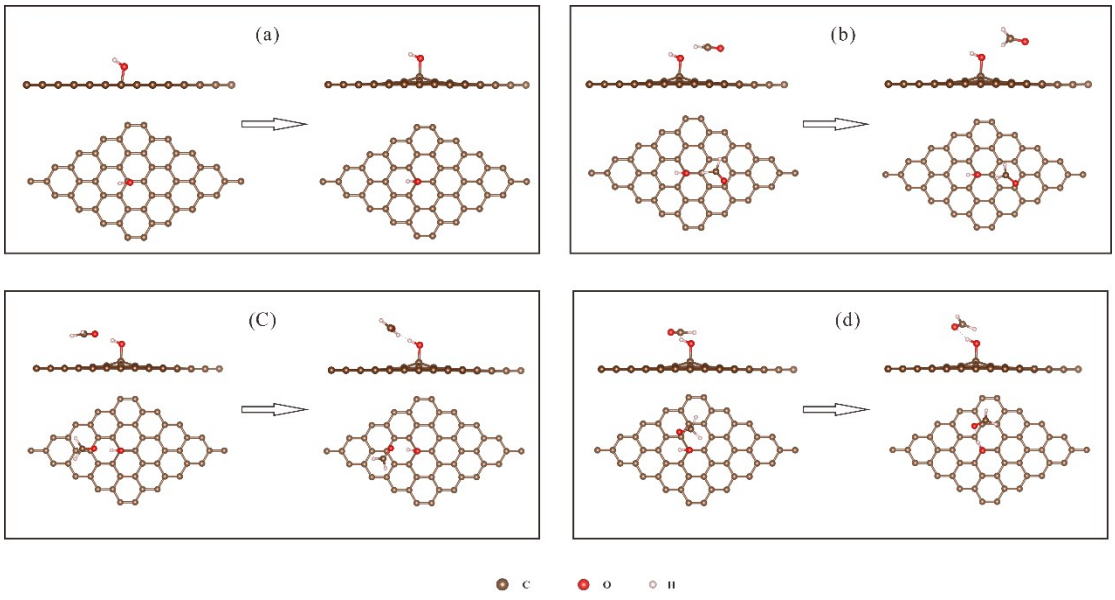

Fig. S4 (a) The model of rGO with individual hydroxyl group (rGO-OH); (b-d) the adsorption structure of HCHO on rGO with hydroxyl group. The left of the arrow is the initial structure, while the right is the optimized structure.

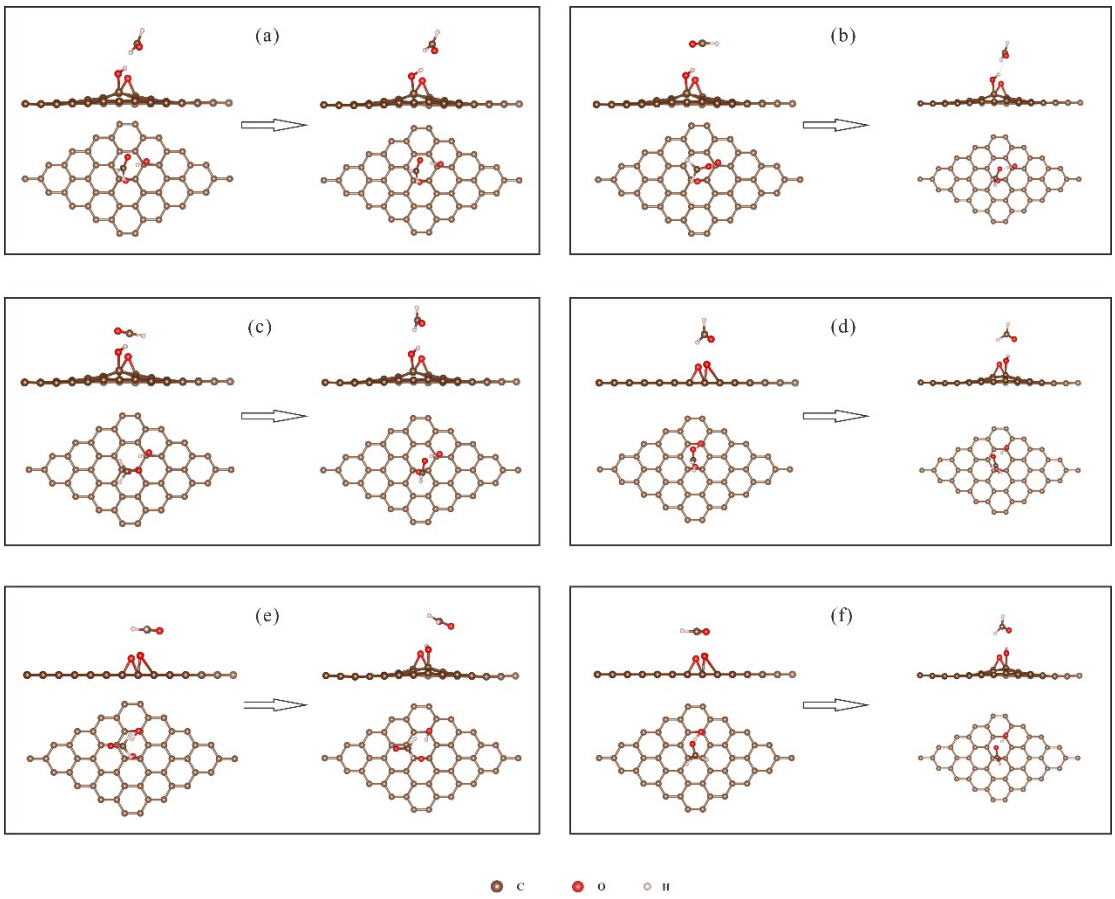

Fig. S5 The adsorption structure of HCHO on rGO with hydroxyl group and epoxide. The left of the arrow is the initial structure, while the right is the optimized structure.

Table S2 The adsorption energy (E_{ads}) and charge transfer (ΔQ) of HCHO molecule adsorbed on rGO with hydroxyl group and epoxide.

		E_{ads} (meV)	ΔQ *(e)*	atom[a]	orientation[b]
1	'rGO-O_OH'	230	0.078	H&O	d
2		186	0.051	H&O	p
3		166	0.042	C&O	p
4	'rGO-O__OH'	177	0.059	H&O	d
5		77	0.007	H&H	p
6		139	0.045	C&O	p

[a] The atom of HCHO molecule close to the oxygen groups, H&H means the two H atom are close to the O atoms of surface. [b] The label d and p mean that the C=O bond of HCHO

molecule pointing down (d) and parallel to the surface (p), starting from C atom.

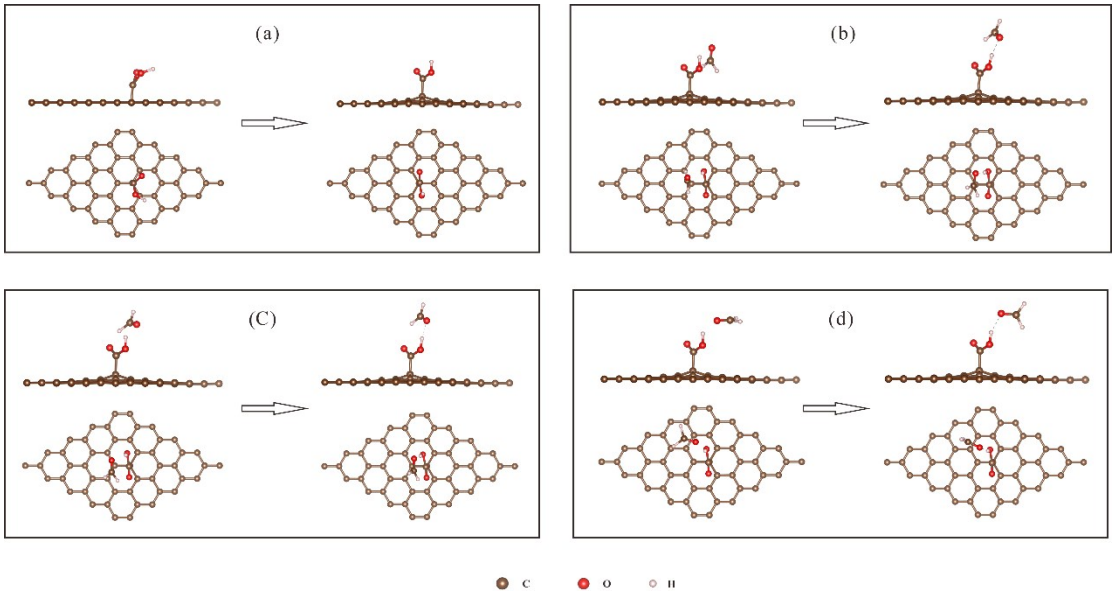

Fig. S6 (a) The model of rGO with carboxyl group; (b-d) the adsorption structure of HCHO on rGO with carboxyl group. The left of the arrow is the initial structure, while the right is the optimized structure.

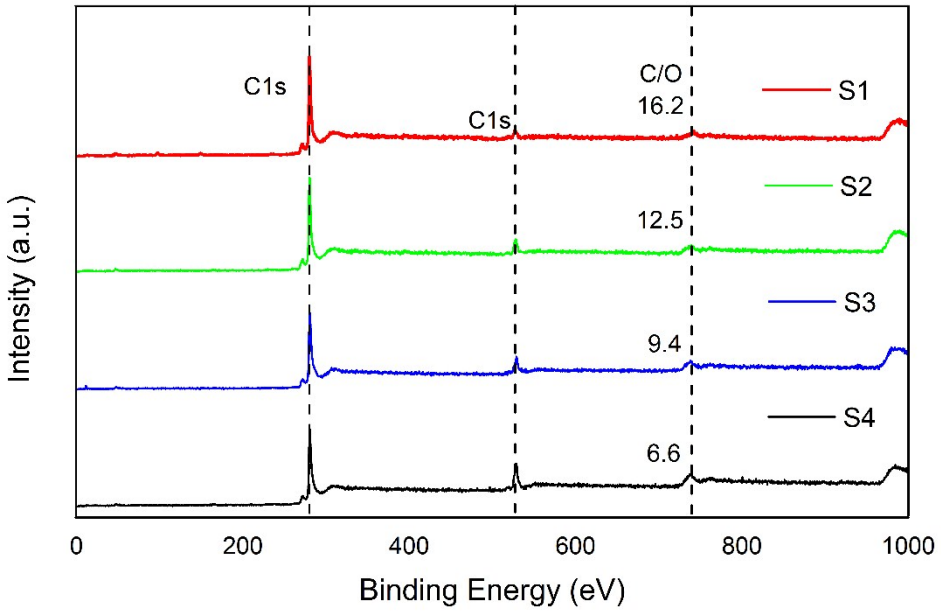

Fig.S7 The XPS spectra of S1, S2, S3, and S4.