Electronic Supplementary Material (ESI) for RSC Advances.

Oxidation of SO_2 and NO by epoxy groups on graphene oxides: The role of the hydroxyl group

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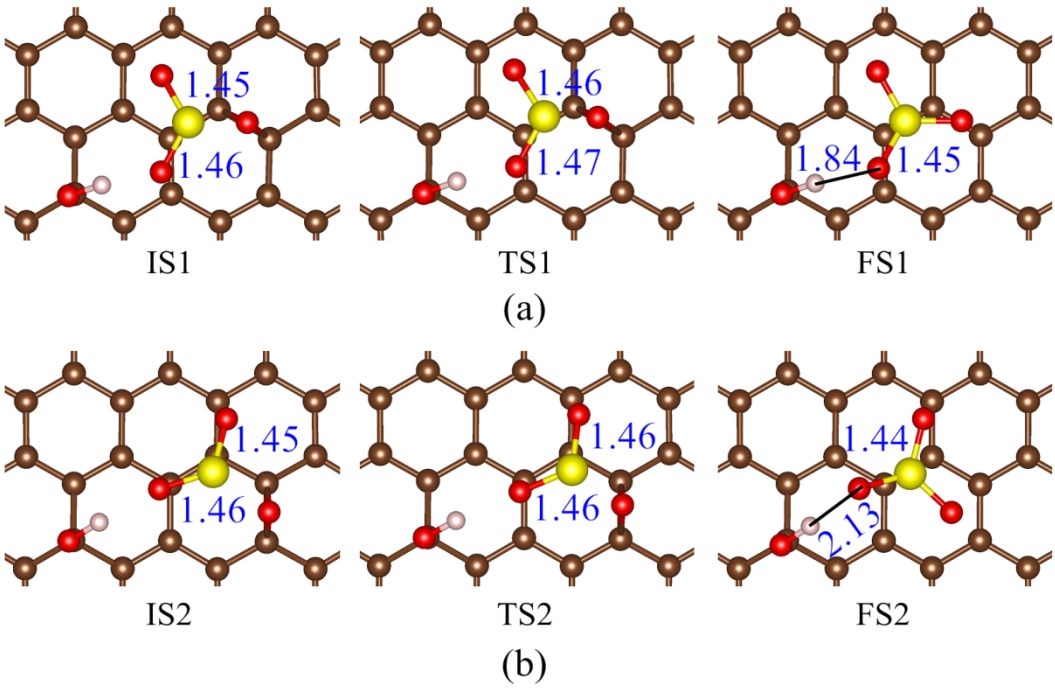


Figure S1 Topviews of MEPs for SO_2 oxidation on (a) HO_OGP1 and (b) HO_OGP2. Since the FS1 is energetic favorable to FS2 by 0.03 eV, only the FS1 is reported as the final state in Figure 2 in the manuscript.

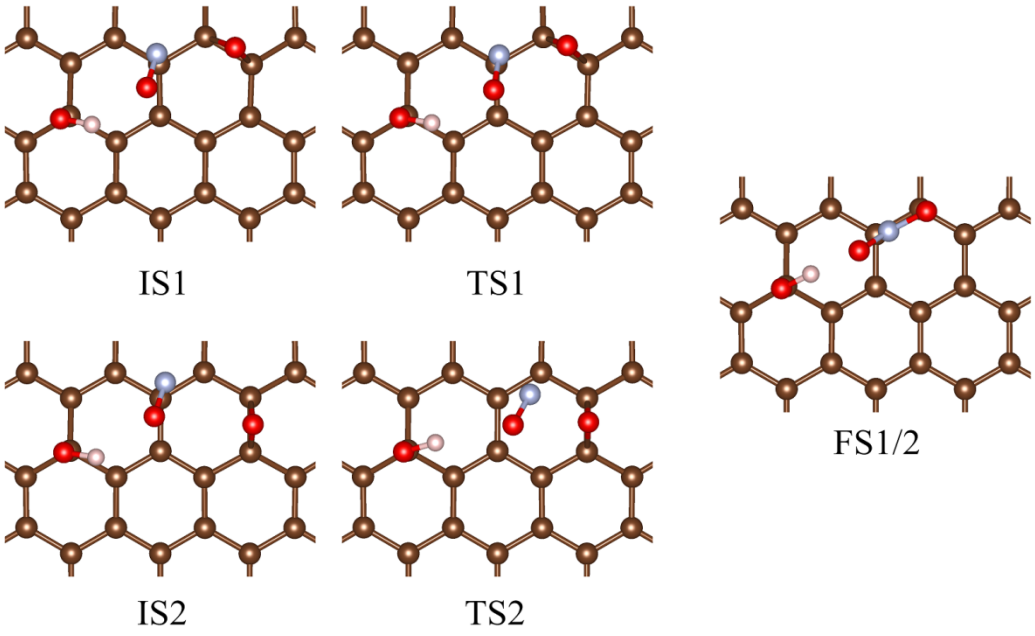


Figure S2 Topviews of MEPs for NO oxidation on (a) HO_OGP1 and (b) HO_OGP2.

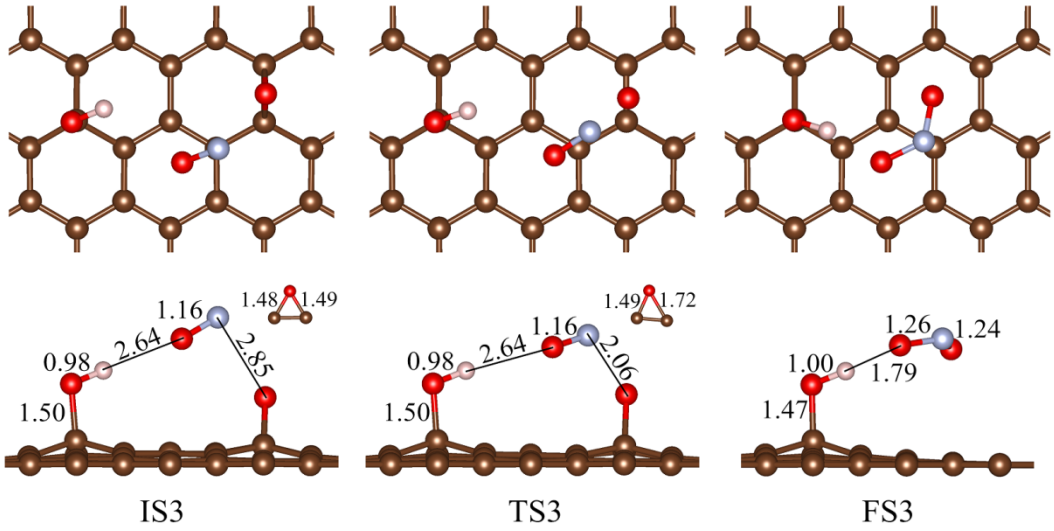


Figure S3 Top and side views of an alternative MEP for NO oxidation on HO_OGP2. The charge difference plot of the IS is shown in Figure 6d in the manuscript. The adsorption energies for IS3 and FS3 are –0.14 and –0.64 eV, respectively. The oxidation barrier is 0.13 eV. For the MEP for NO oxidation on HO_OGP2 discussed in Figure 4 and Figure S3, the adsorption energies of IS2 and FS2 are –0.25 (see Table 1 in the manuscript) and –0.80 eV (see Table S2), respectively. Subsequently, only the more stable configurations and the oxidation process related are reported in the manuscript.

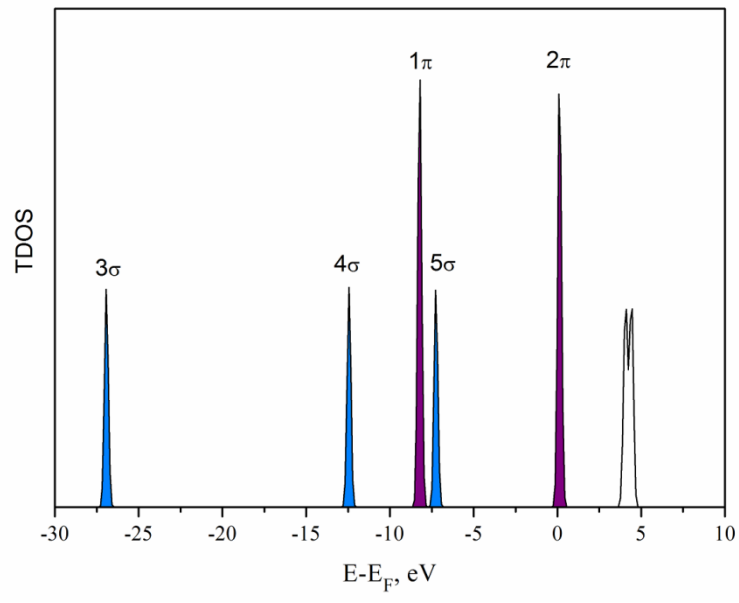
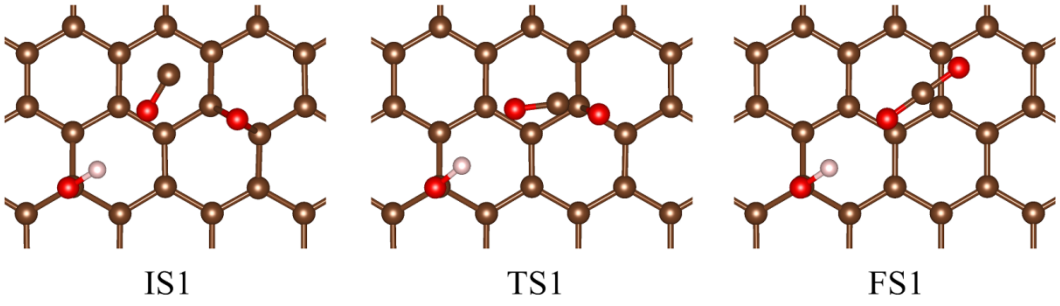
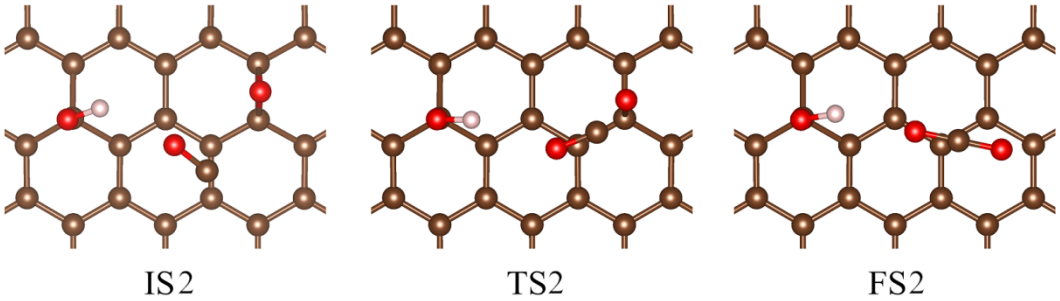


Figure S4 Orbit-projected density of states (PDOS) of adsorbed NO molecule. Each of the σ orbits is filled with 2e. The 1π is filled with 4e. Because the 2π is filled with 1e, three fourth of which is unoccupied, it is located at the Fermi level.



(a)



(b)

Figure S5 Topviews of MEPs for CO oxidation on (a) HO_OGP1 and (b) HO_OGP2. Since the FS1 is energetic favorable to FS2 by 0.1 eV, only the FS1 is reported as the final state in Figure 3 in the manuscript.

Table S1 Adsorption energy (in eV) recheck for optB88-vdW and spin polarization.

Entries	non-spin polarized		spin polarized	
	D2	optB88-vdW	D2	m(μ_B)
SO_2/OGP	−0.30	−0.46	−0.30	−0.0003
SO_2/HO_OGP1	−0.40	−0.55	−0.40	+0.0084
SO_2/HO_OGP2	−0.45	−0.61	−0.45	+0.0000
SO_2/2HO_OGP	−0.58	−0.72	−0.58	−0.0001
NO/OGP	−0.10	/	−0.10	+1.0053
NO/HO_OGP1	−0.54	/	−0.29	+0.2030
NO/HO_OGP2	−0.25	/	−0.20	+0.9714

Table S2 Oxidation barrier (in eV) recheck for spin polarization.

Reactions	non-spin polarized	spin polarized
SO_2/OGP→SO_3/GP	−0.21	−0.207
NO/HO_OGP1→NO_2/HO_GP	−0.11	−0.119

Table S3 Adsorption energy and charge transfer for the adsorption of SO_3, NO_2 and CO_2 on GP,

HO_GP and 2HO_GP surfaces. Only the values of the most stable configurations are collected.

Conf.	ΔE_{ads}, eV	Δq, e
SO_3/GP	–0.31	0.080
SO_3/HO_GP	–0.46	0.290
SO_3/2HO_GP	–0.51	0.400
NO_2/GP	–0.49	0.344
NO_2/HO_GP	–0.80	0.407
CO_2/GP	–0.15	0.015
CO_2/HO_GP	–0.20	0.010