Supporting Information for

Double graphic-N doping for enhanced catalytic activity of carbocatalysts

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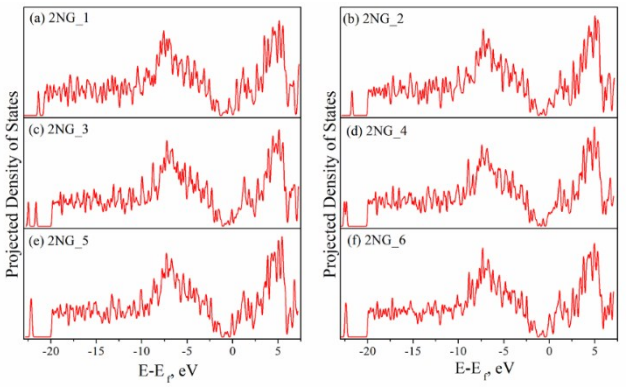

Figure S1. Total density of states (TDOS) of different double GrN atoms doped graphene.

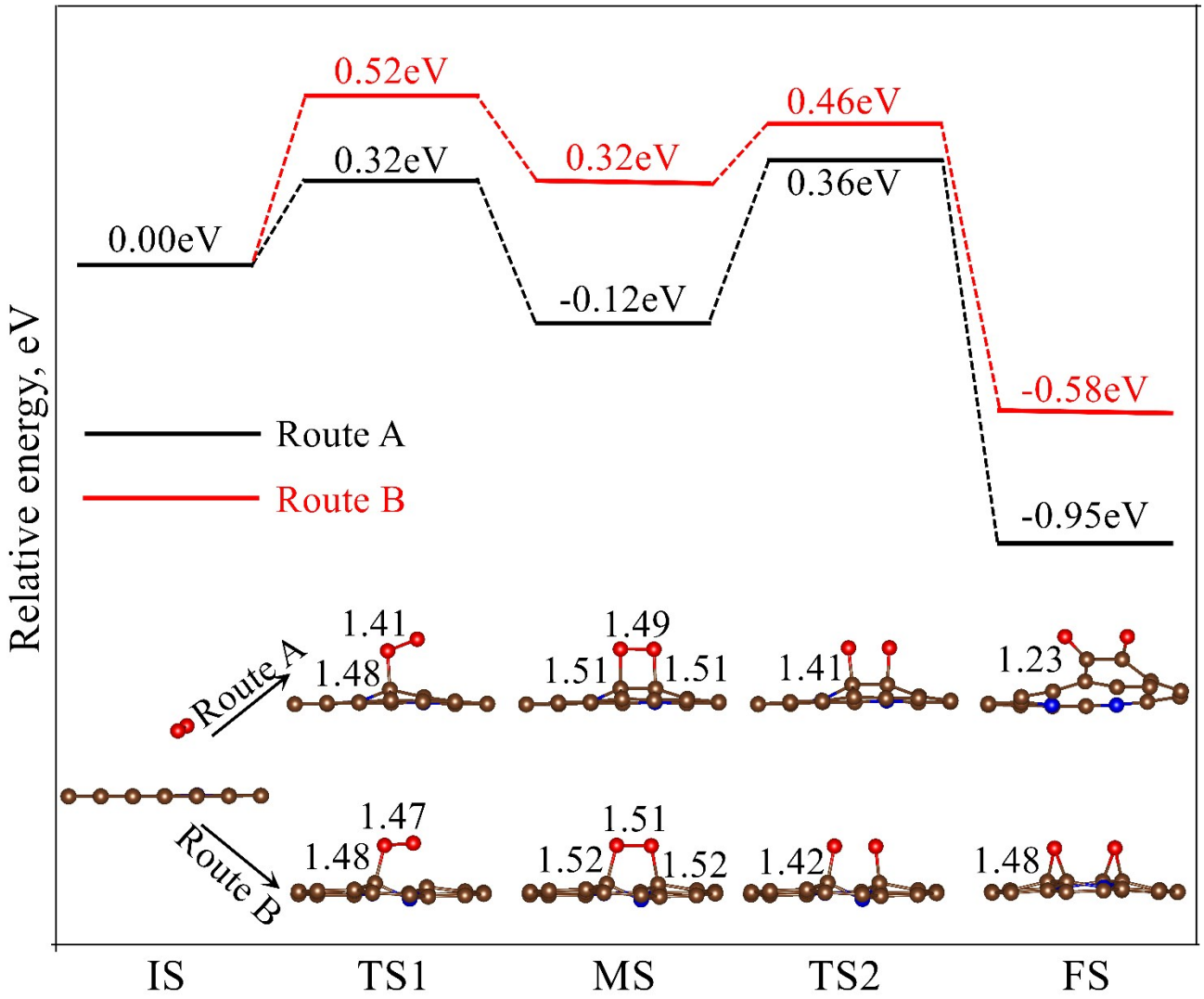

Figure S2. Minimum energy pathway (MEP) of O_2 dissociation reactions (ODR) by 2NG_3.

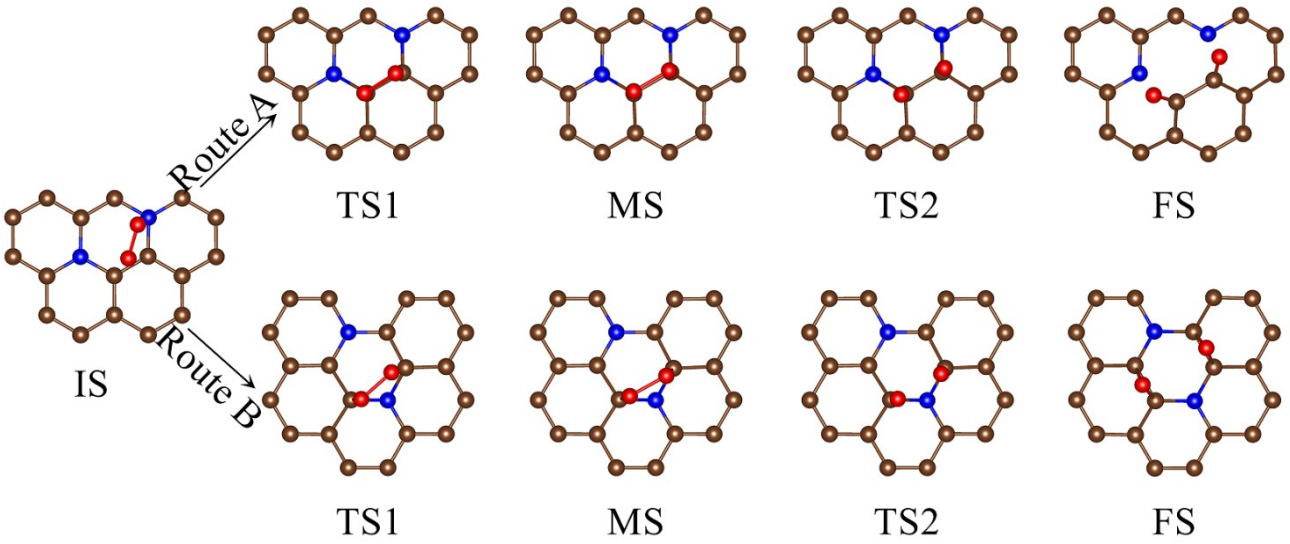

Figure S3. Top view of minimum energy pathway (MEP) of O_2 dissociation reactions (ODR) by 2NG_3.

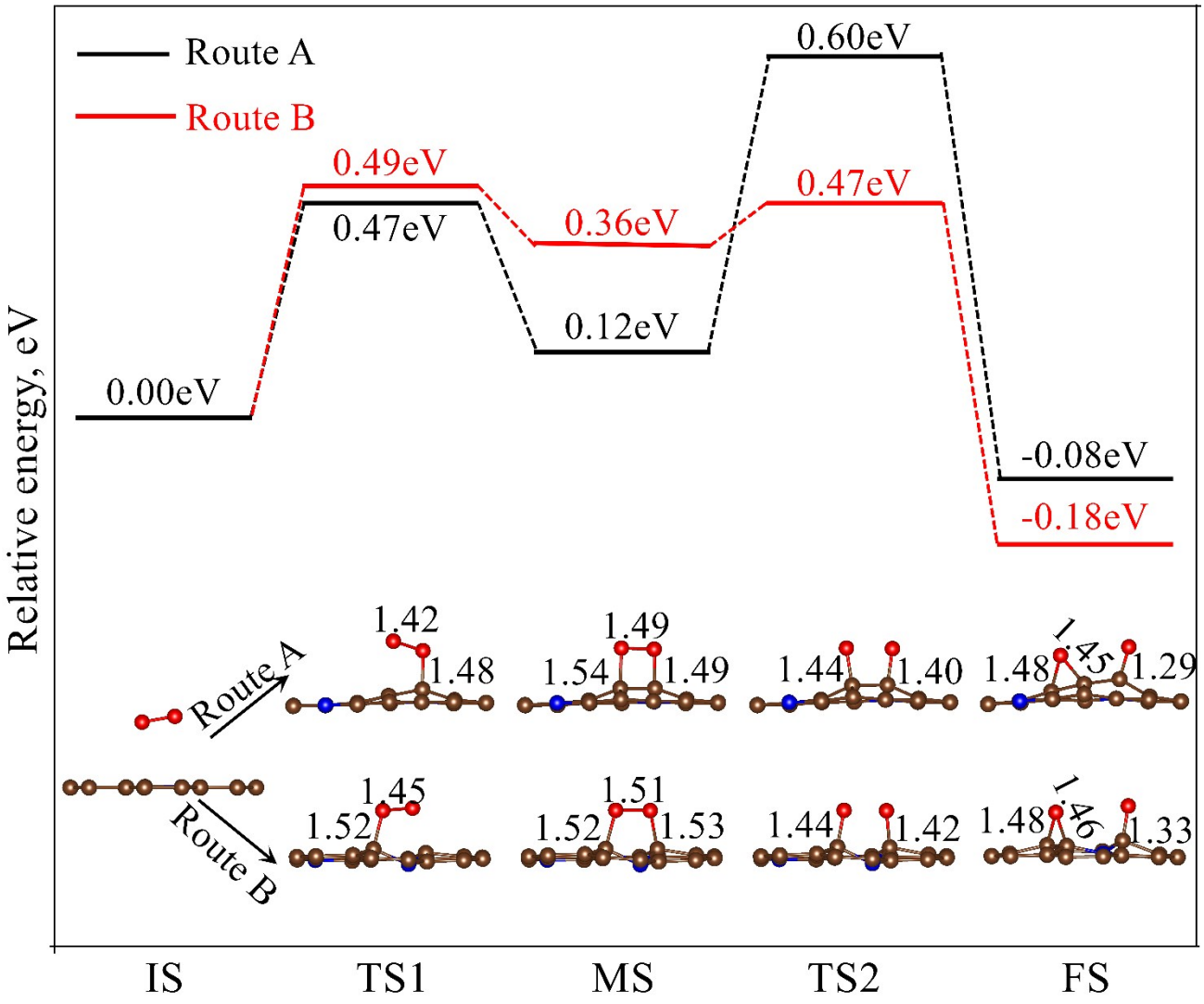

Figure S4. Minimum energy pathway (MEP) of O_2 dissociation reactions (ODR) by 2NG_5. Red, blue and brown spheres depict O, N and C atoms. All lengths are given in Å.

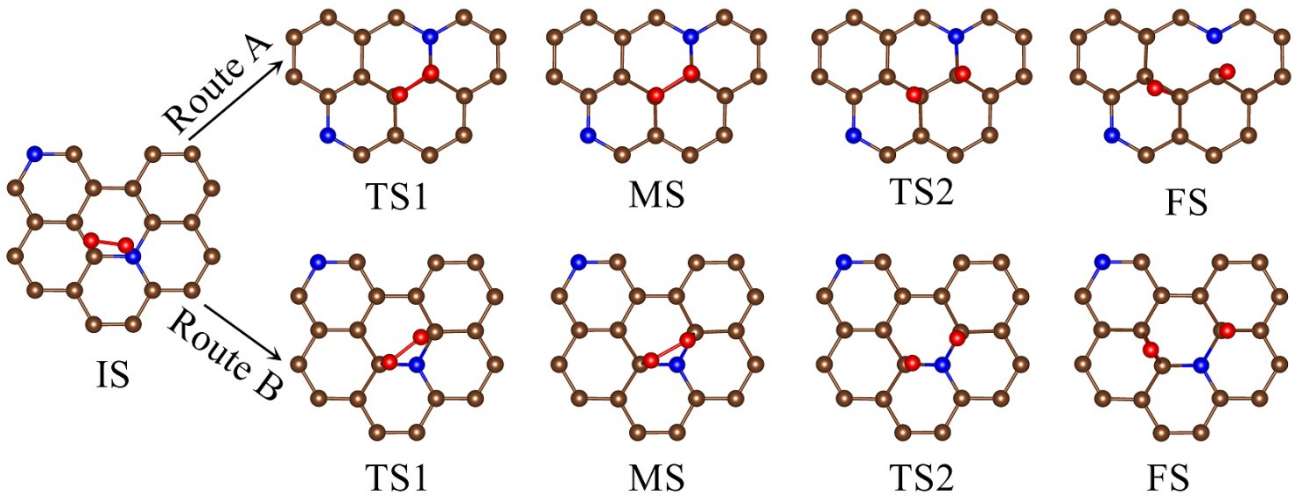

Figure S5. Top view of minimum energy pathway (MEP) of O_2 dissociation reactions (ODR) by 2NG_5.

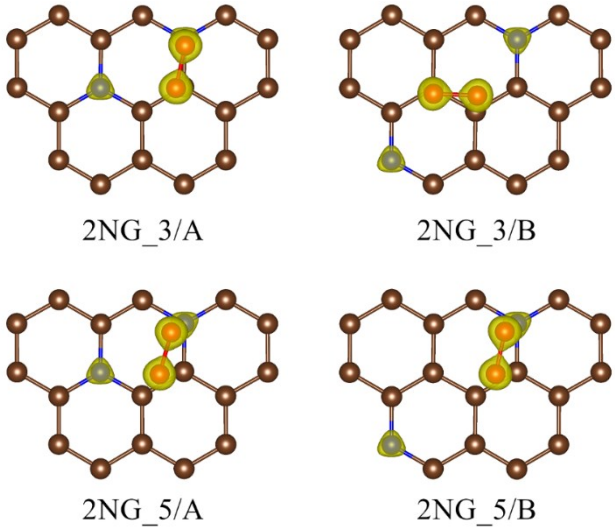

Figure S6. Spin charge density of O_2 adsorbed on different double GrN atoms doped graphene. All the absorbed oxygen molecules are in triple state and in ground state.

Table S1. Summary of the Calculated Results for O_2 Adsorption on Different Surfaces

configuration	$d_{O\text{-}O}$[a] (Å)	$d_{O\text{-}C}$[b] (Å)	$d_{O\text{-}N}$[b] (Å)	$d_{O\text{-}sur}$[b] (Å)	Δq_{IS}[c] (*e*)	Δq_{TS}[c] (*e*)
2NG_3/A	1.29	2.58	2.69	2.68	0.41	1.21
2NG_3/B	1.29	2.47	2.64	2.68	0.35	0.82
2NG_5/A	1.28	2.55	3.24	2.58	0.41	0.83
2NG_5/B	1.28	2.54	2.73	2.52	0.36	0.78

a: Bond length of the O_2 molecule. b: Distance between O, the closest C/N atom on the surface and the surface. c: Bader effective charge for the O_2 molecule. Δq = Bader population – valence electrons.

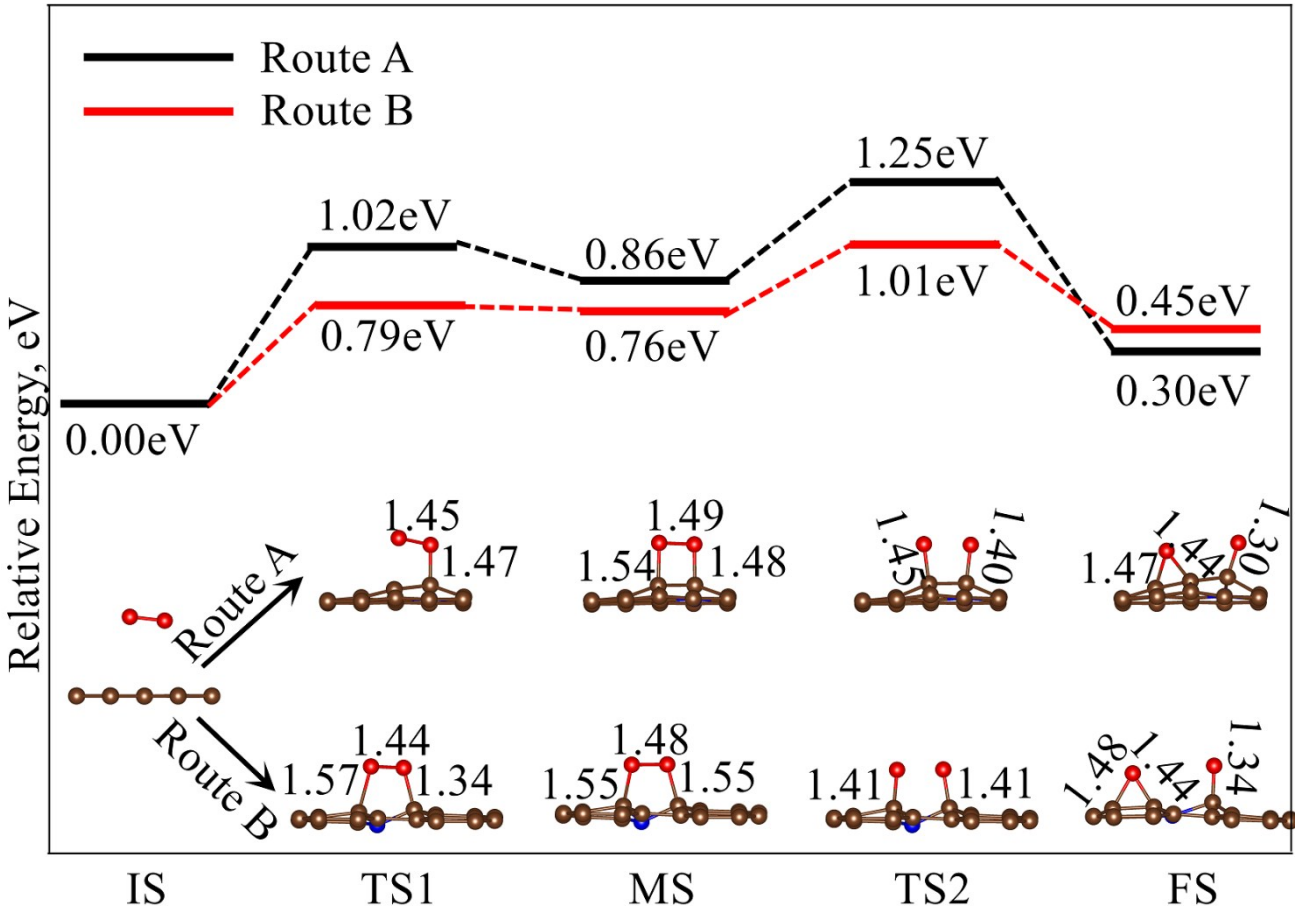

Figure S7. Minimum energy pathway (MEP) of O_2 dissociation reactions (ODR) by NG. Red, blue and brown spheres depict O, N and C atoms. All lengths are given in Å.

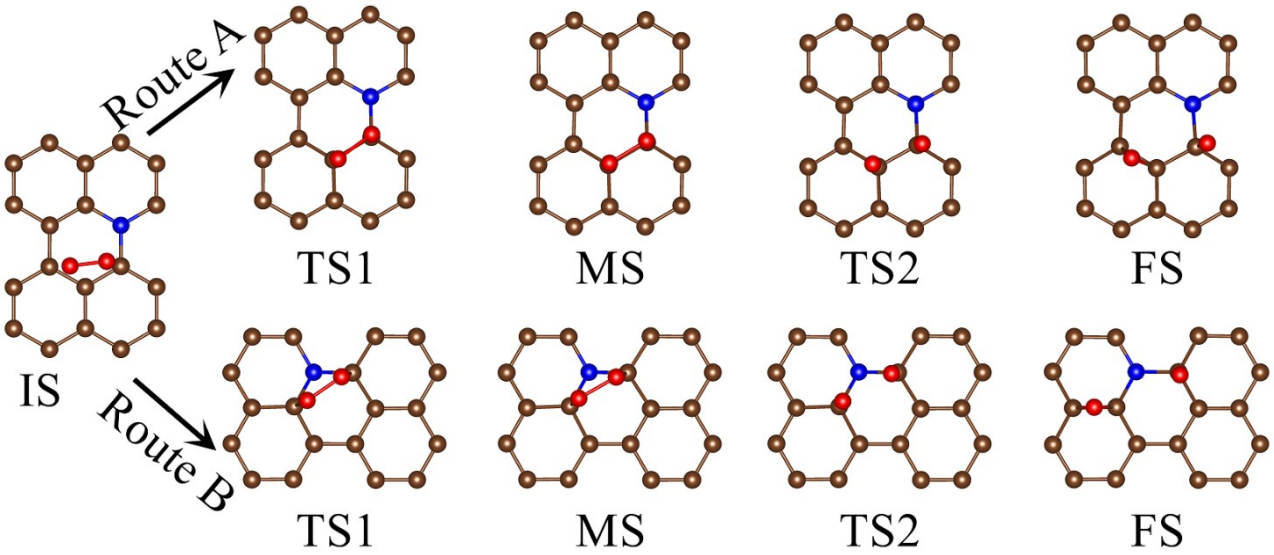

Figure S8. Top view of minimum energy pathway (MEP) of O_2 dissociation reactions (ODR) by NG.

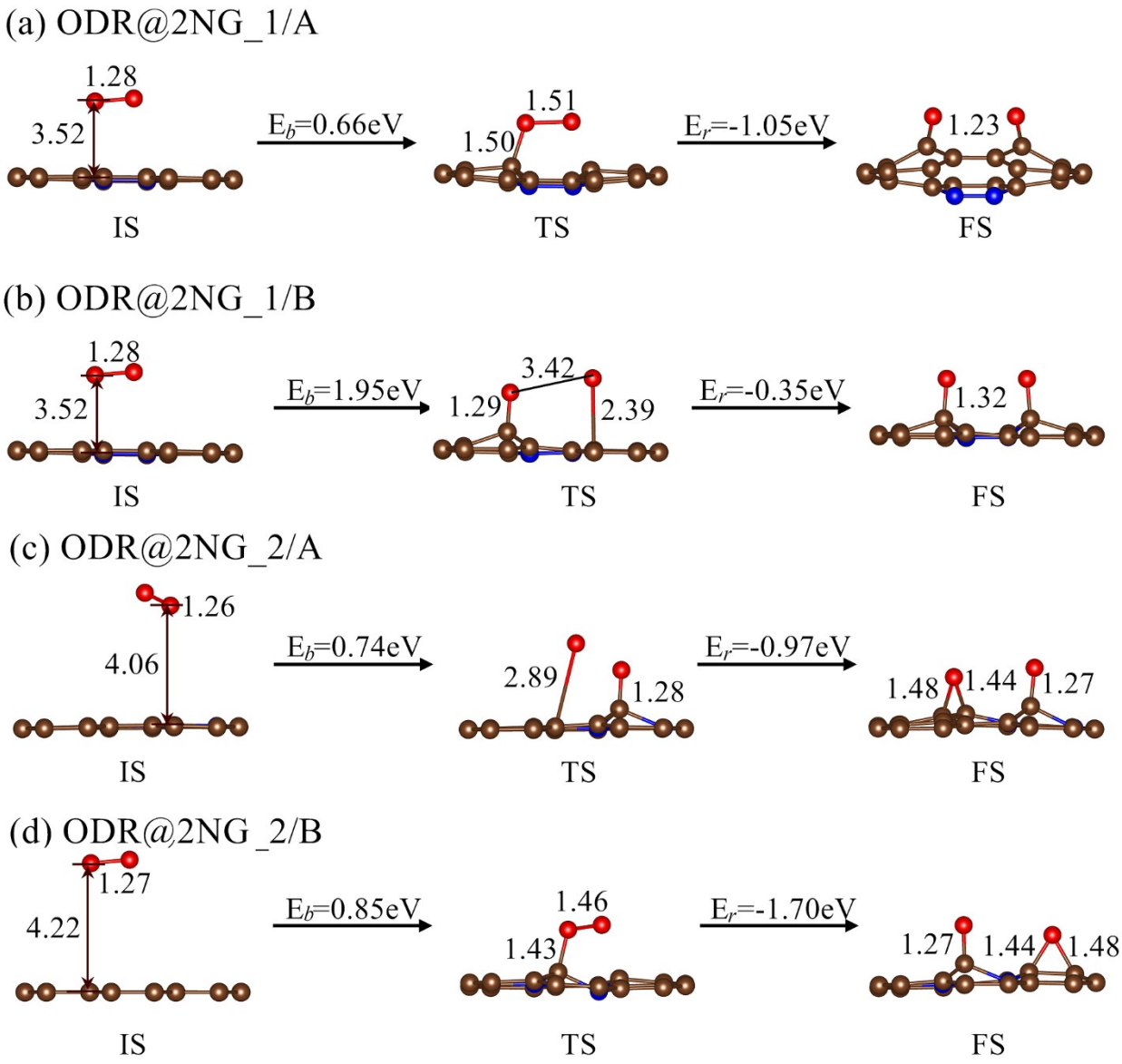

Figure S9 Minimum energy pathway (MEP) of O_2 dissociation reaction on 2NG_1 (a and b), 2NG_2 (c~d). E_b and E_r stand for the energy barrier and reaction energy respectively. Red, blue and brown spheres depict O, N and C atoms. All lengths are given in Å.

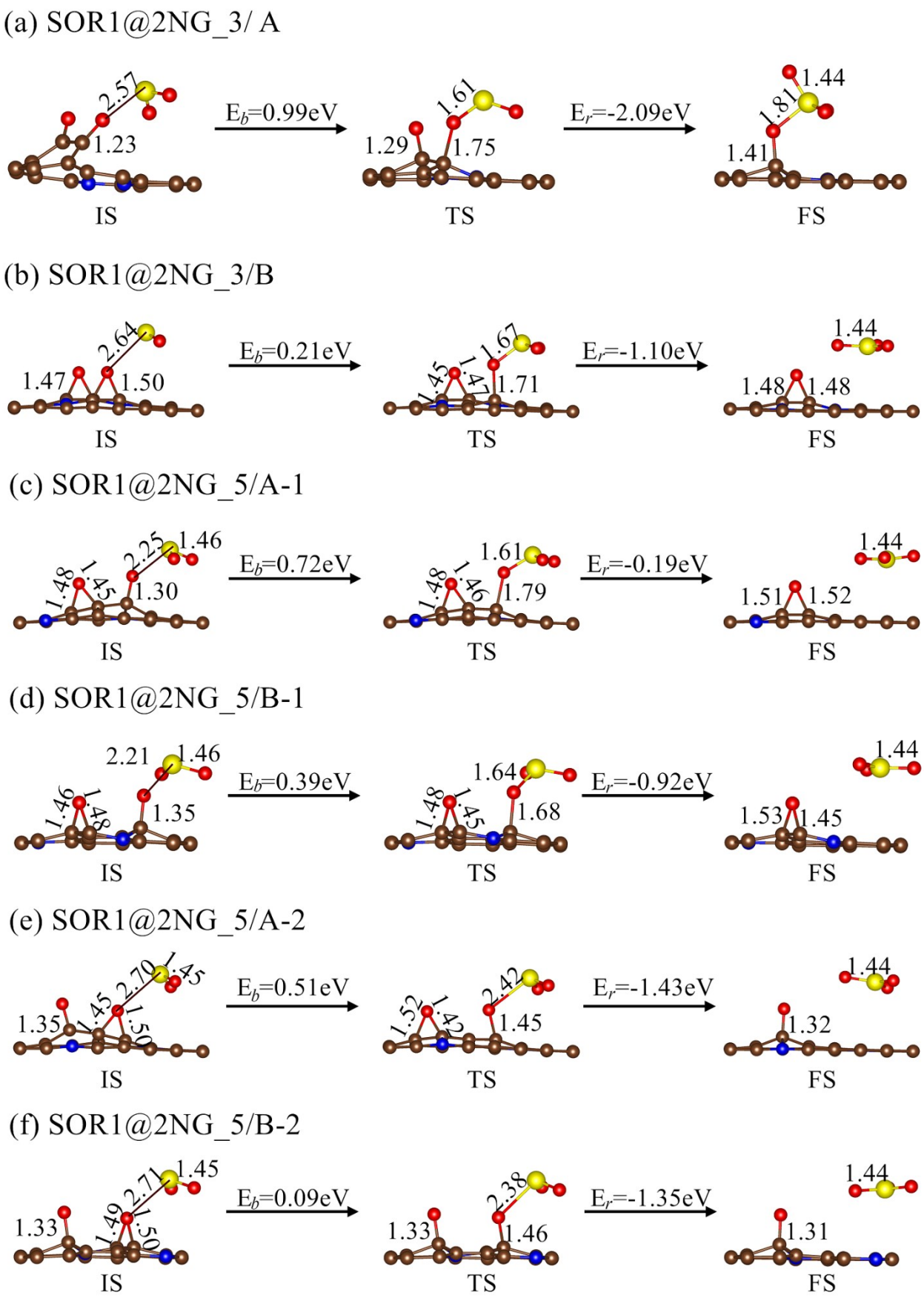

Figure S10. Minimum energy pathway (MEP) of SO_2 oxidation reactions 1 (SOR1) by

2NG_3 (a and b), 2NG_5 (c~f). E_b and E_r stand for the energy barrier and reaction energy respectively. Red, blue and brown spheres depict O, N and C atoms. All lengths are given in Å.

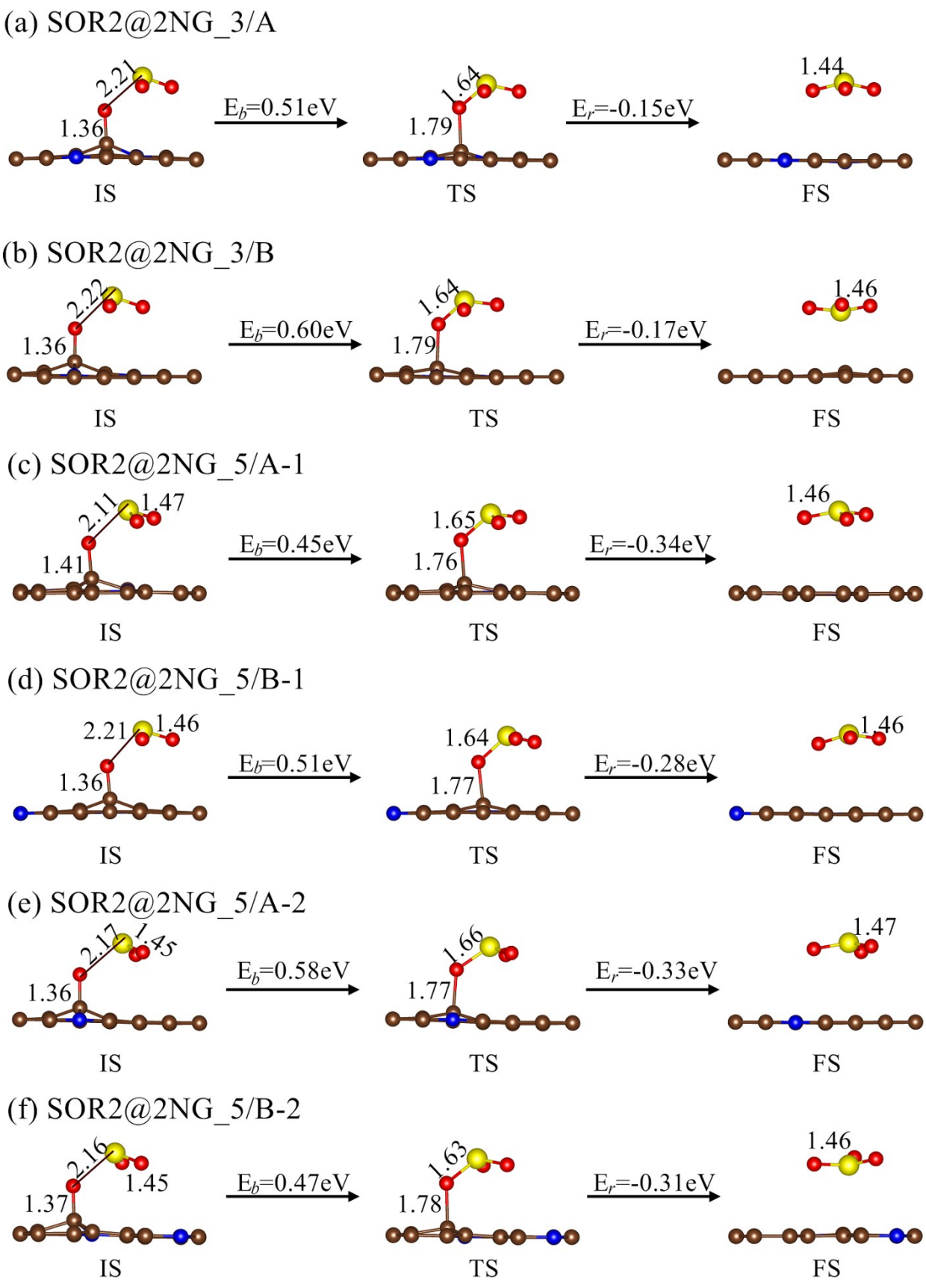

Figure S11. Minimum energy pathway (MEP) of SO_2 oxidation reactions 2 (SOR2) by

2NG_3 (a and b), 2NG_5 (c~f). E_b and E_r stand for the energy barrier and reaction energy respectively. Red, blue and brown spheres depict O, N and C atoms. All lengths are given in Å.

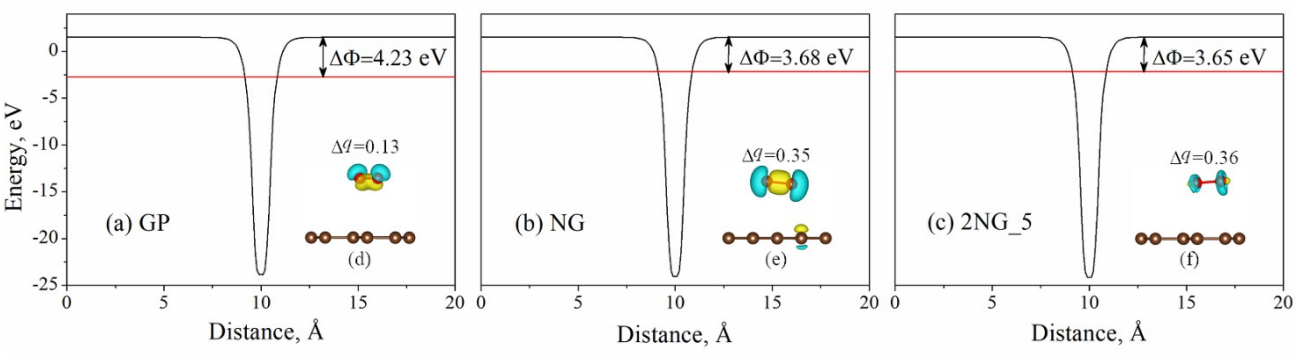

Figure S12. Work function of different surface. (a): GP; (b): NG; (c): 2NG_5. The red line stands for Fermi level. Inset: Charge difference for O2 adsorbed on different surface. The isosurfaces is set to 0.005 eV/Å^3.

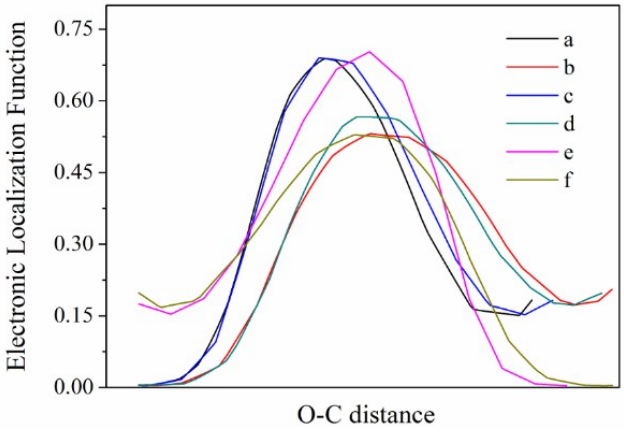

Figure S13. Electron localization function (ELF) between O-C for oxygen groups on GrN-doped graphene. (a): carbonyl in 2NG_3; (b): epoxy in 2NG_3; (c): carbonyl in 2NG_3/A; (d): epoxy in 2NG_3/B; (e): carbonyl in 2NG_5/A; (f): epoxy in 2NG_5/B.