Electronic Supplementary Information For Promoting Mechanism of Pyridine N Doped Carbocatalyst for SO_2 Oxidation

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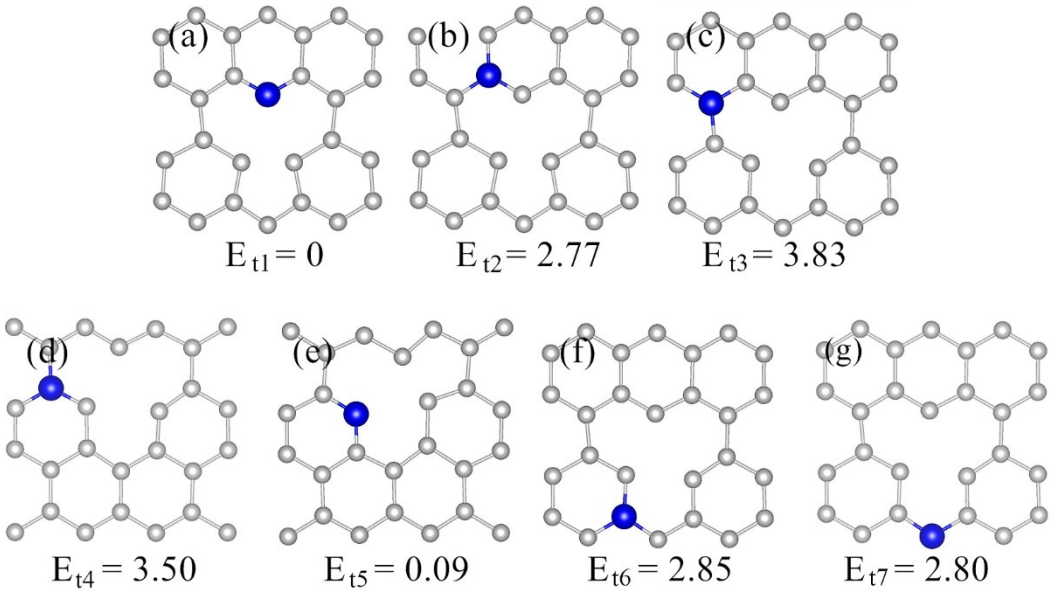


Figure S1 Possible structures and total energy (E_t) of a single N doped VG at different sites. The total energy of the most stable configuration in (a) is set to be 0 eV as reference. Blue and grey spheres represent N, C atoms, respectively. All energy is given in eV and positive means heat absorption.

Table S1 Total doping energy (E_d) and substep doping energy (E_s) for PyN.

Conf.	E_d, eV	E_s, eV
1N_VG	-2.06	-2.06
2N_VG	-2.44	-0.89
3N_VG	-4.01	-1.50
1N_DVG	-0.09	-0.09
2N_DVG	-1.55	-1.04
3N_DVG	-1.72	-0.77
4N_DVG	-3.56	-1.73

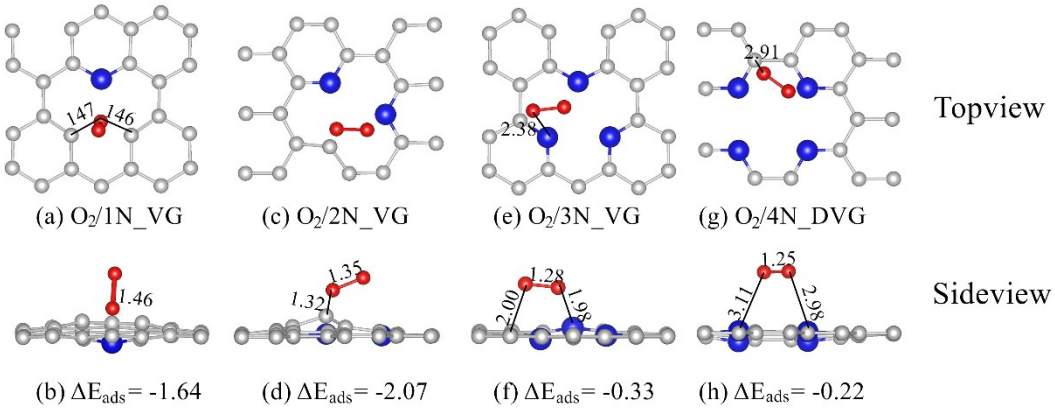


Figure S2 Optimized adsorption structures of O_2 on different PyN doped surfaces. Red, blue and grey spheres represent O, N and C atoms. All lengths and energy are given in Å and eV, respectively. Negative means heat release

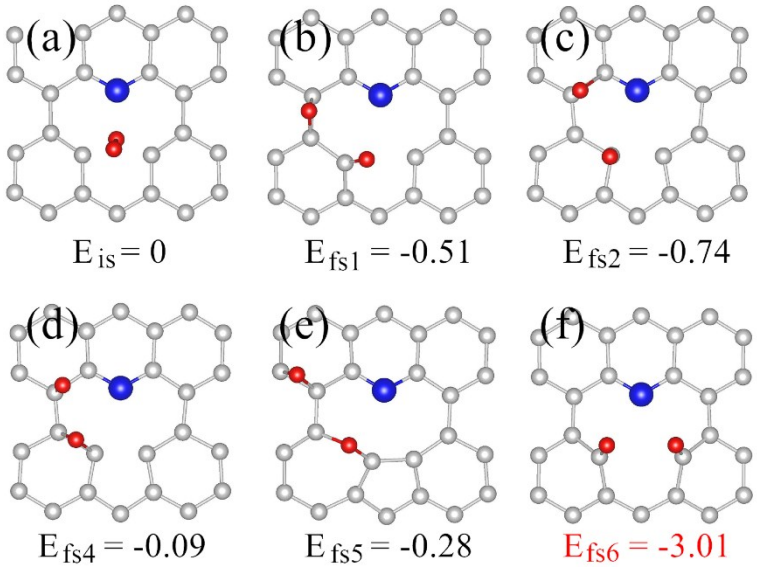


Figure S3 Possible structures and energy of O_2 dissociation on 1N_VG. Total energy of the initial configuration in (a) is set to be 0 eV as reference. The color coding is the same as Fig. S3. Energy is given in eV and negative means heat release.

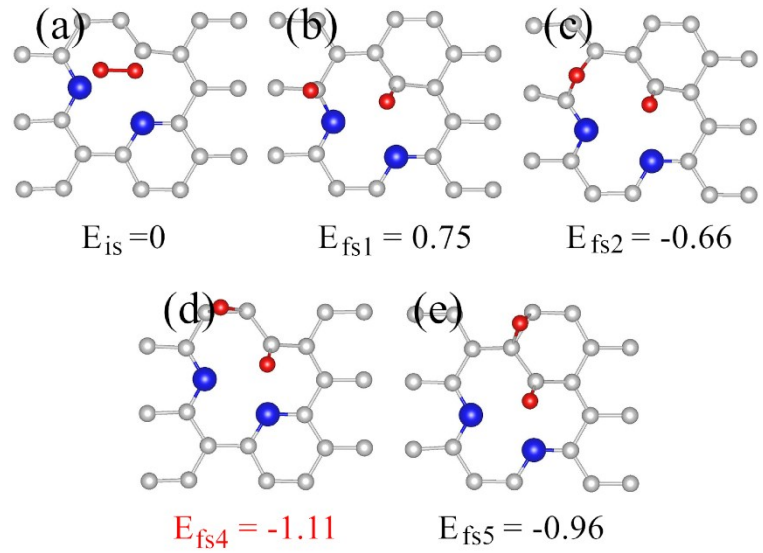


Figure S4 Possible structures and energy of O_2 dissociation on 2N_VG. Total energy of the initial configuration in (a) is set to be 0 eV as reference. The color coding is the same as Fig. S3. Energy is given in eV and negative means heat release.

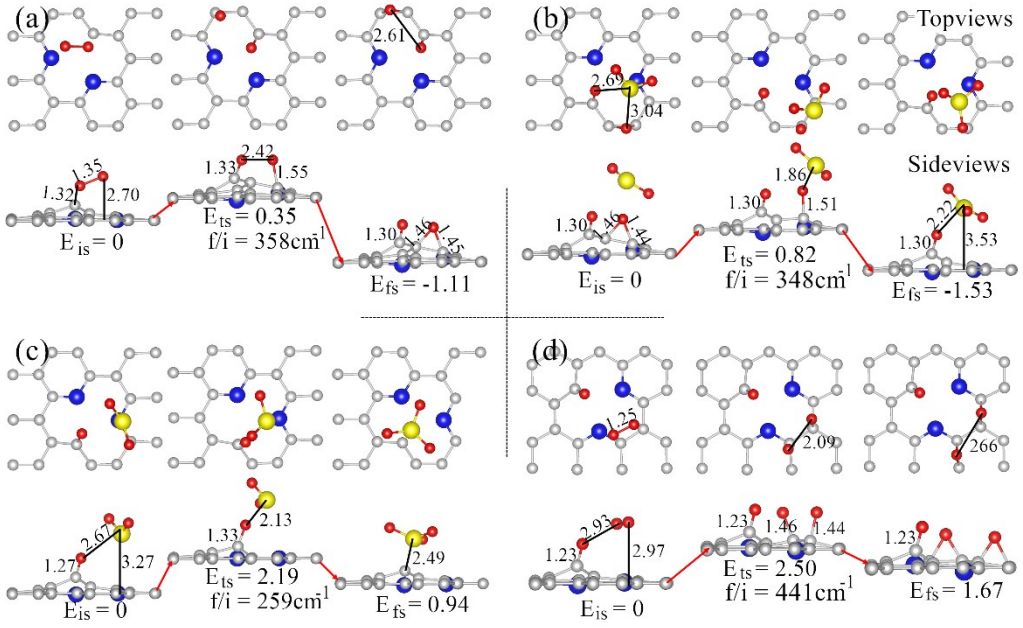
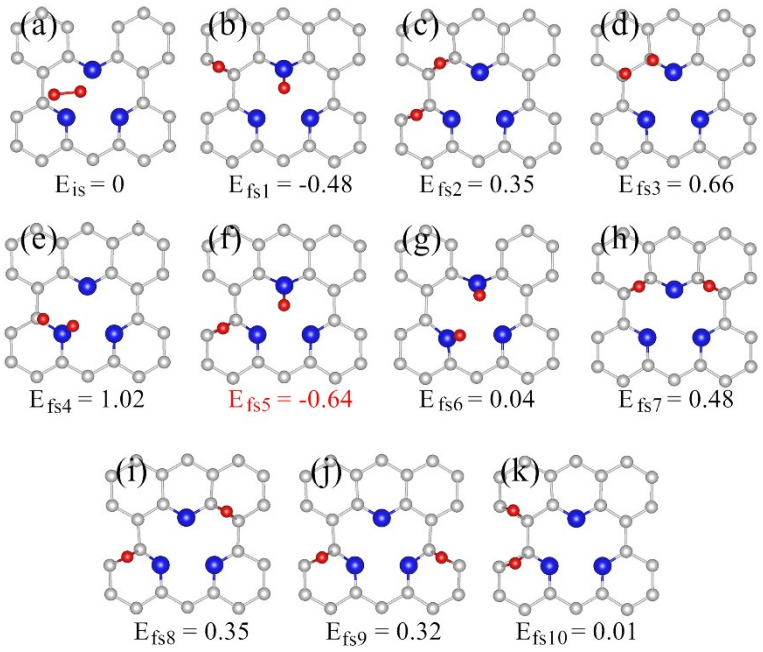


Fig. S5 Catalytic oxidation of SO_2 on 2N_VG: (a) ODR1, (b) SOR1, (c) SOR2 and (d) ODR2. Blue, red, yellow and grey spheres represent N, O, S and C atoms. All the lengths and energy are given in Å and eV, respectively. Fig. S5d tested the second ODR on 1O/2N_VG, the results indicates that O_2 is thermodynamically unfavorable, with an energy barrier of 1.60 eV and net energy of 1.03eV.



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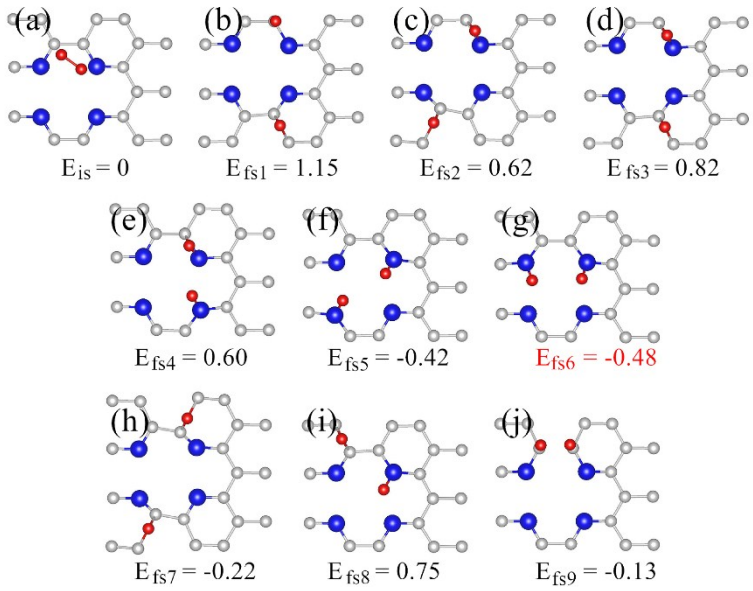
42 **Figure S6** Possible structures and energy of O_2 dissociation on 3N_VG. Total energy of the
43 initial configuration in (a) is set to be 0 eV as reference. The color coding is the same as Fig. S3.
44 Energy is given in eV and negative means heat release.



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46 **Figure S7** Possible structures and energy of O_2 dissociation on 4N_DVG. Total energy of the
47 initial configuration in (a) is set to be 0 eV as reference. The color coding is the same as Fig. S3.
48 Energy is given in eV and negative means heat release.