SUPPORTING INFORMATION

Dissociation of O_2 and Its Reactivity on O/S doped Graphene

Meiling Hou[1], Wanglai Cen[2,3]*, Fang Nan[4], Jianjun Li[1,3], Yinghao Chu[1,3]*, Huaqiang Yin[1,3]

1. College of Architecture and Environment, Sichuan University, Chengdu, 610065, P. R. China;

2. Institute of New Energy and Low Carbon Technology, Sichuan University, Chengdu, 610065, P. R. China;

3. National Engineering Research Center for Flue Gas Desulfurization, Chengdu, 610065, P. R. China;

4. Sichuan Electric Design and Consulting Company, Chengdu, 610094, P. R. China.

Corresponding Author:

Dr. Wanglai Cen (cenwanglai@163.com)

Dr. Yinghao Chu(chuyinghao@scu.edu.cn)

Tel/Fax: +86 28 85403016

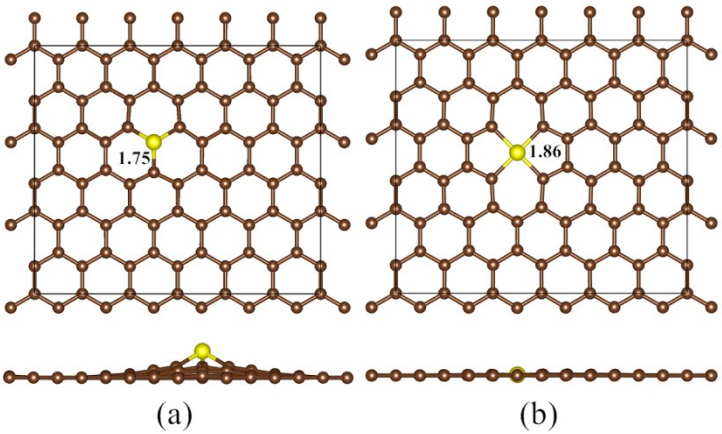

Figure S1 Geometric structures of SG in different doping mode. (a): S atom replaced one C atom (SG1); (b): S atom replaced two C atoms (SG2). Yellow and brown spheres denote S and C atoms, respectively. The length of C-S bonds were given in Å.

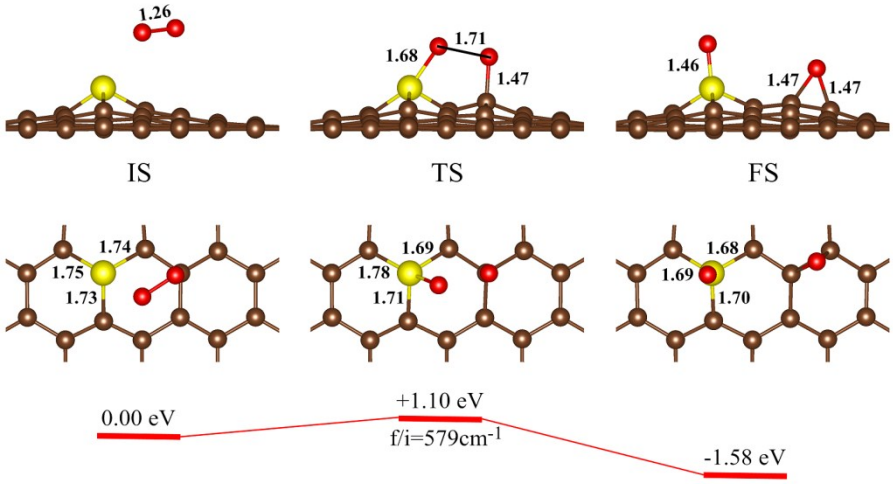

Figure S2 Minimum energy pathway (MEP) for the dissociation of O_2 on SG1. All the lengths are given in Å. It denotes that the dissociation of O_2 on SG1 is not kinetically preferable.

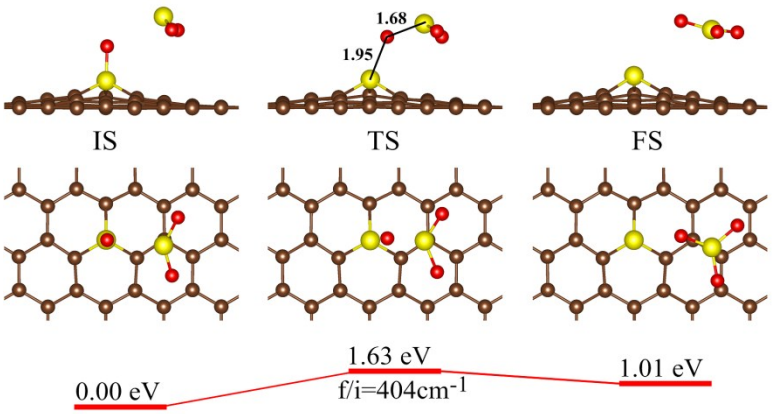

Figure S3 Oxidation of SO_2 on SG1. It denotes that the oxidation is not kinetically and thermodynamically preferable.

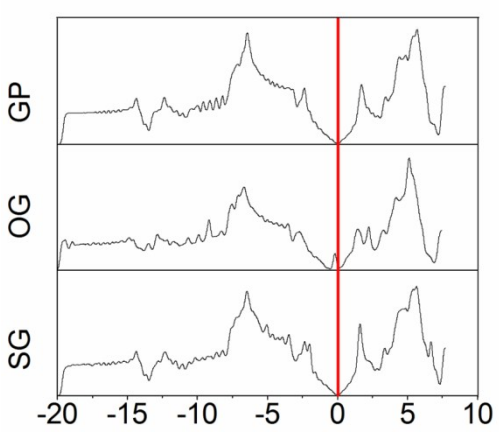

Figure S4 Density of states (DOS) analysis for different surfaces.

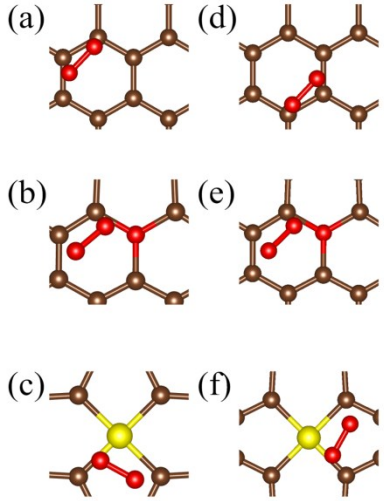

Figure S5 Top view of adsorption configurations of O_2 on GP, OG and SG surfaces. Spin polarization was ignored in (a)-(c), while it was included for (d)-(f). All the distances are given in Å.

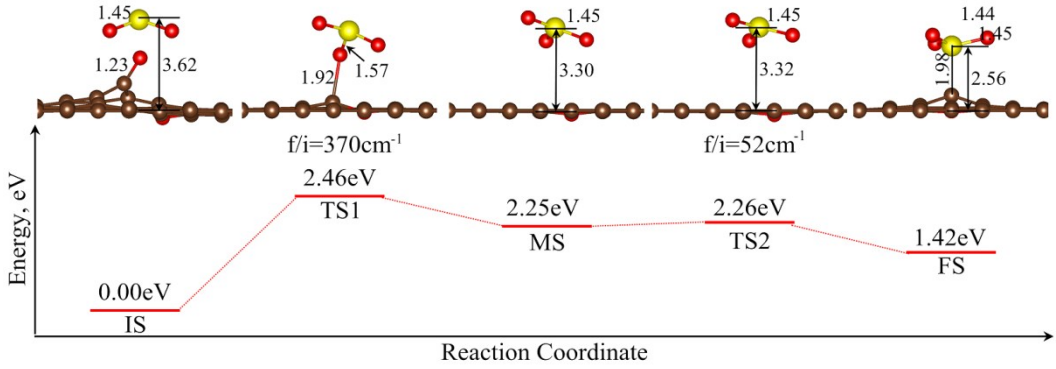

Figure S6 Minimum energy pathway (MEP) for the oxidation of SO_2 by 1O_OG. All the lengths are given in Å.

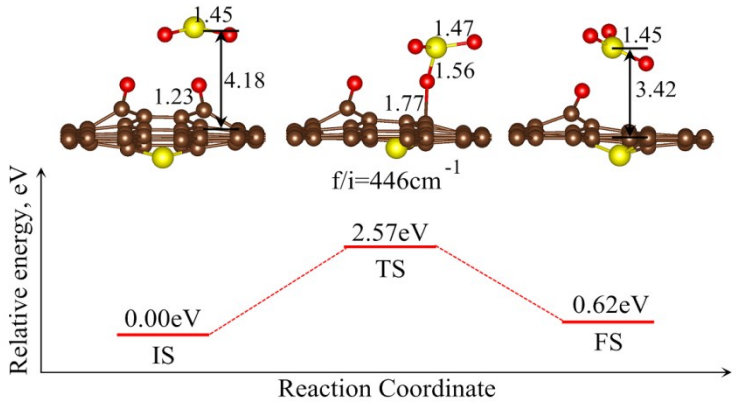

Figure S7 Minimum energy pathway (MEP) for the oxidation of SO_2 by 2O_SG. All the lengths are given in Å.

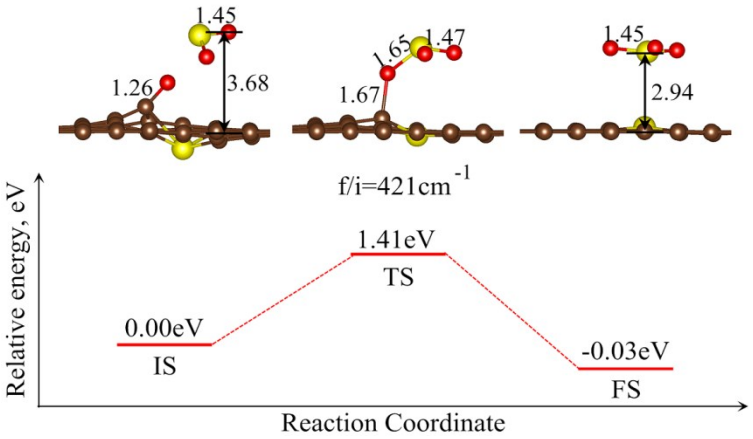

Figure S8 Minimum energy pathway (MEP) for the oxidation of SO_2 by 1O_SG. All the lengths are given in Å.

Table S1 The main energy barriers (E_b) of the O_2 dissociation processes

Reaction	O_2/GP		O_2/SG		O_2/OG	
	NSP[a]	SP[b]	NSP	SP	NSP	SP
E_b, eV	1.78	1.59	0.39	0.19	0.05	0.04