Carbon-Doped Hexagonal Boron Nitride: an Effective Catalyst for Oxidative Desulfurization

Hongping Li [a], Wendi Fu [a], Jie Yin [a], Jinrui Zhang [a], Yujun Li [a], Ding Jiang [b], Naixia Lv [c*], Wenshuai, Zhu [a*]

[a] Institute for Energy Research, School of Chemistry and Chemical Engineering, Jiangsu University, Zhenjiang, 212013, P. R. China

[b] School of Energy and Power Engineering, Jiangsu University, Zhenjiang, 212013, P. R. China

[c] College of Biology and Chemistry, Xingyi Normal University For Nationalities, Xingyi, 562400, P. R. China

***Corresponding author**:

E-mail: xiaoxia791102@163.com (N. X. Lv); zhuws@ujs.edu.cn (W. S. Zhu)

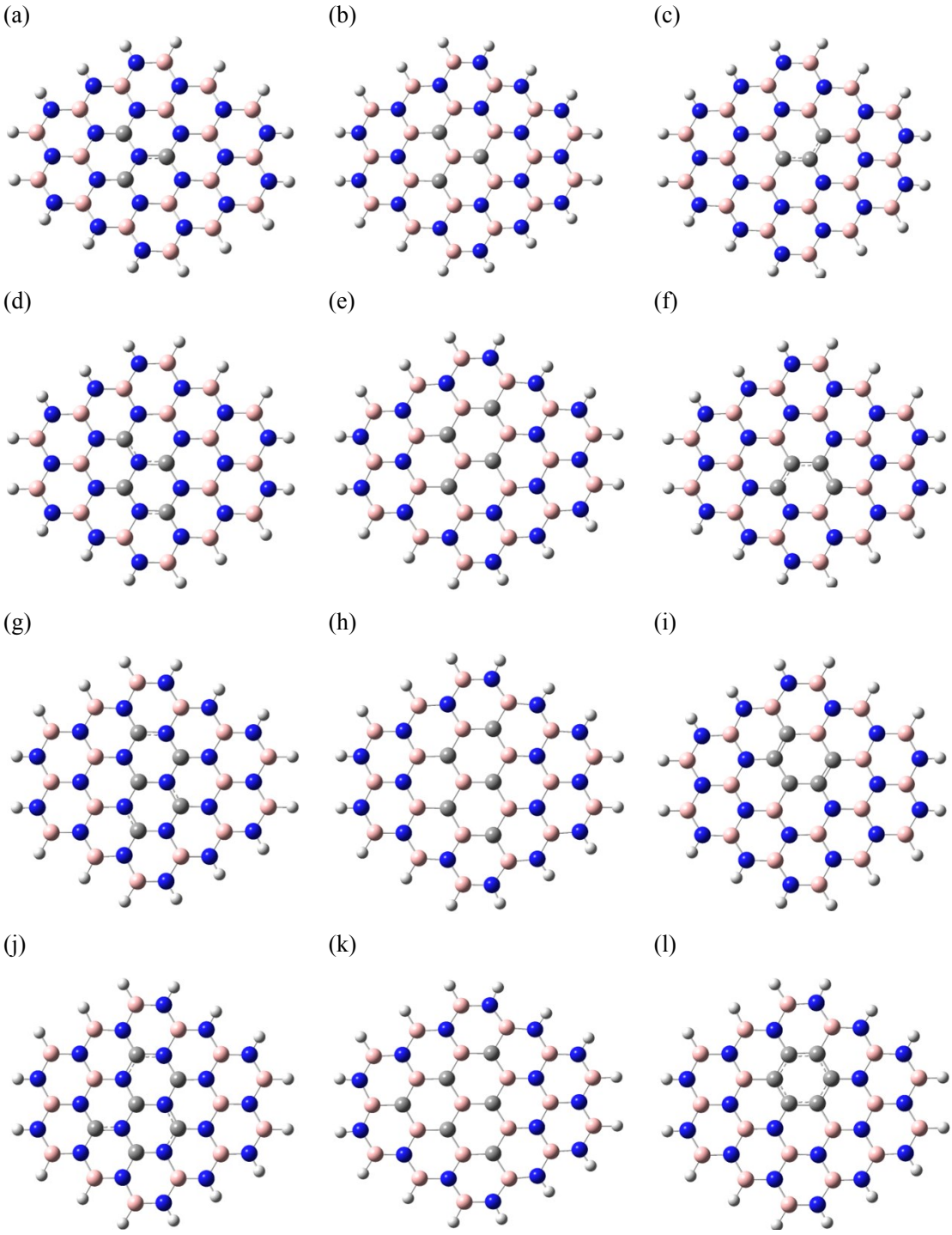

Figure S1. Cluster models for C-doped h-BN sheet (a)C_{3B}, (b) C_{3N}, (c) C_{B2N}, (d) C_{4B}, (e) C_{4N}, (f) C_{2B2N}, (g) C_{5B}, (h) C_{5N}, (i) C_{2B3N}, (j) C_{6B}, (k) C_{6N}, (l) C_{3B3N}.

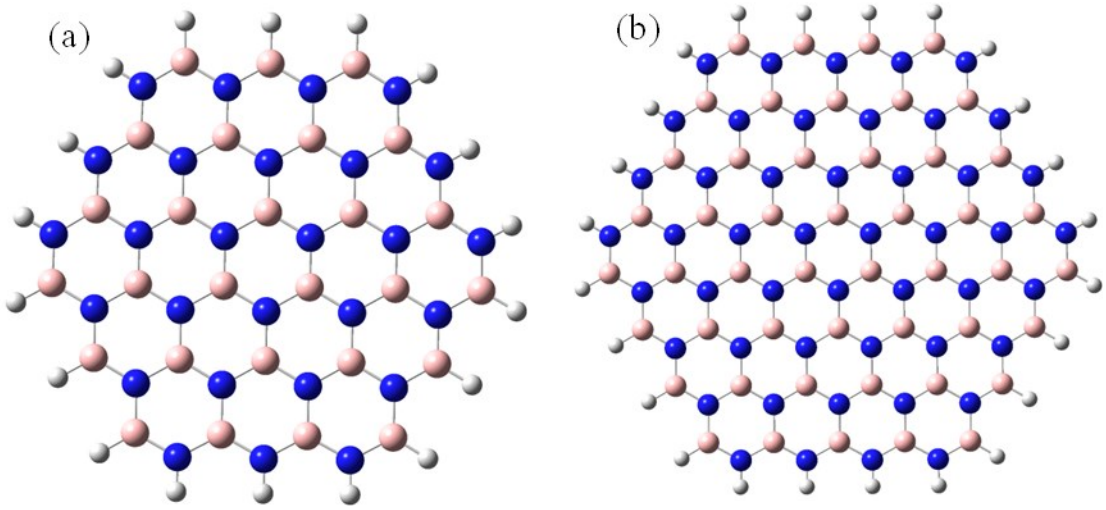

Figure S2. Cluster models for h-BN sheet (a) $B_{27}N_{27}$, (b) $B_{48}N_{48}$

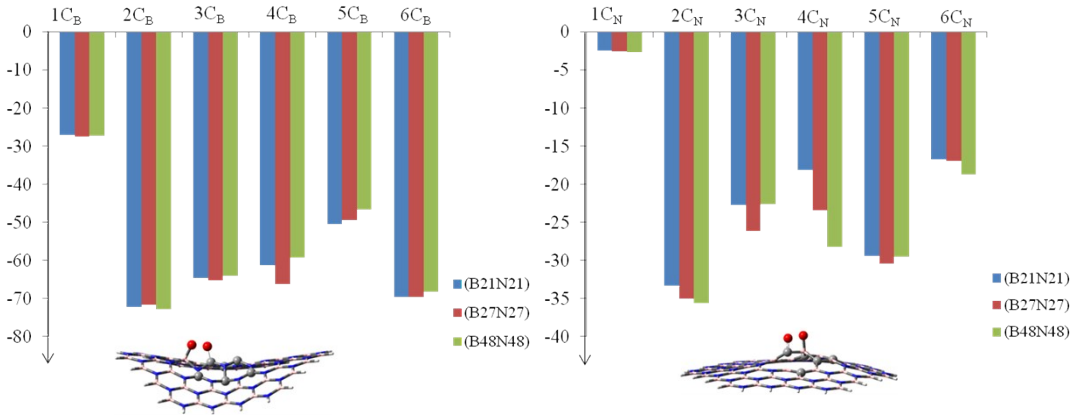

Figure S3. The adsorption energies for O_2 on the different C-doped h-BN models. Left: O_2 on the dispersed C_B surface. Right: O_2 on the dispersed C_N surface.

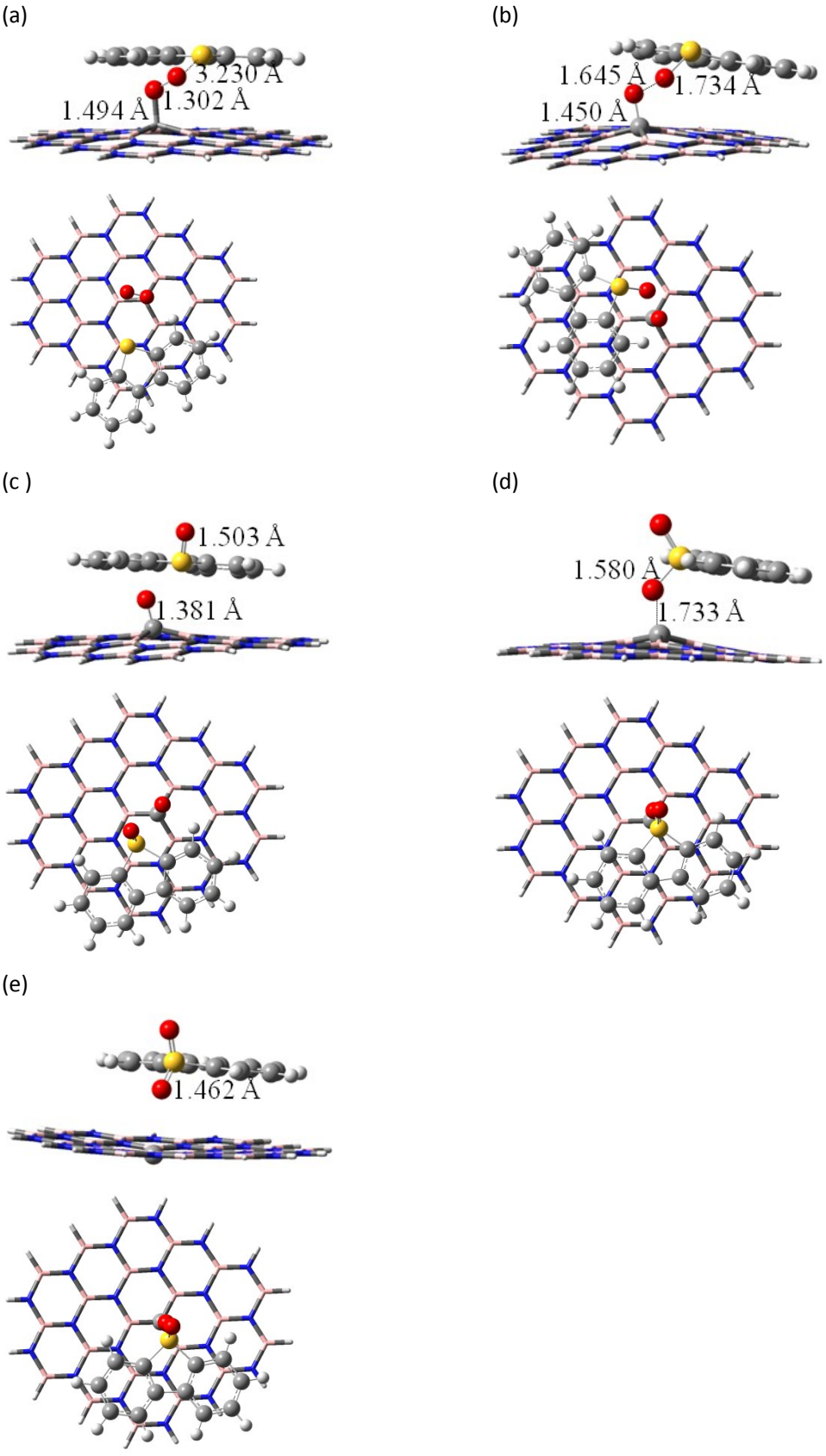

Figure S4 DBT oxidation on C_N model. (a) O_2 and DBT co-adsorption (b)TS1 (c) IM1, DBTO (d) TS2 (e)FS, DBTOO

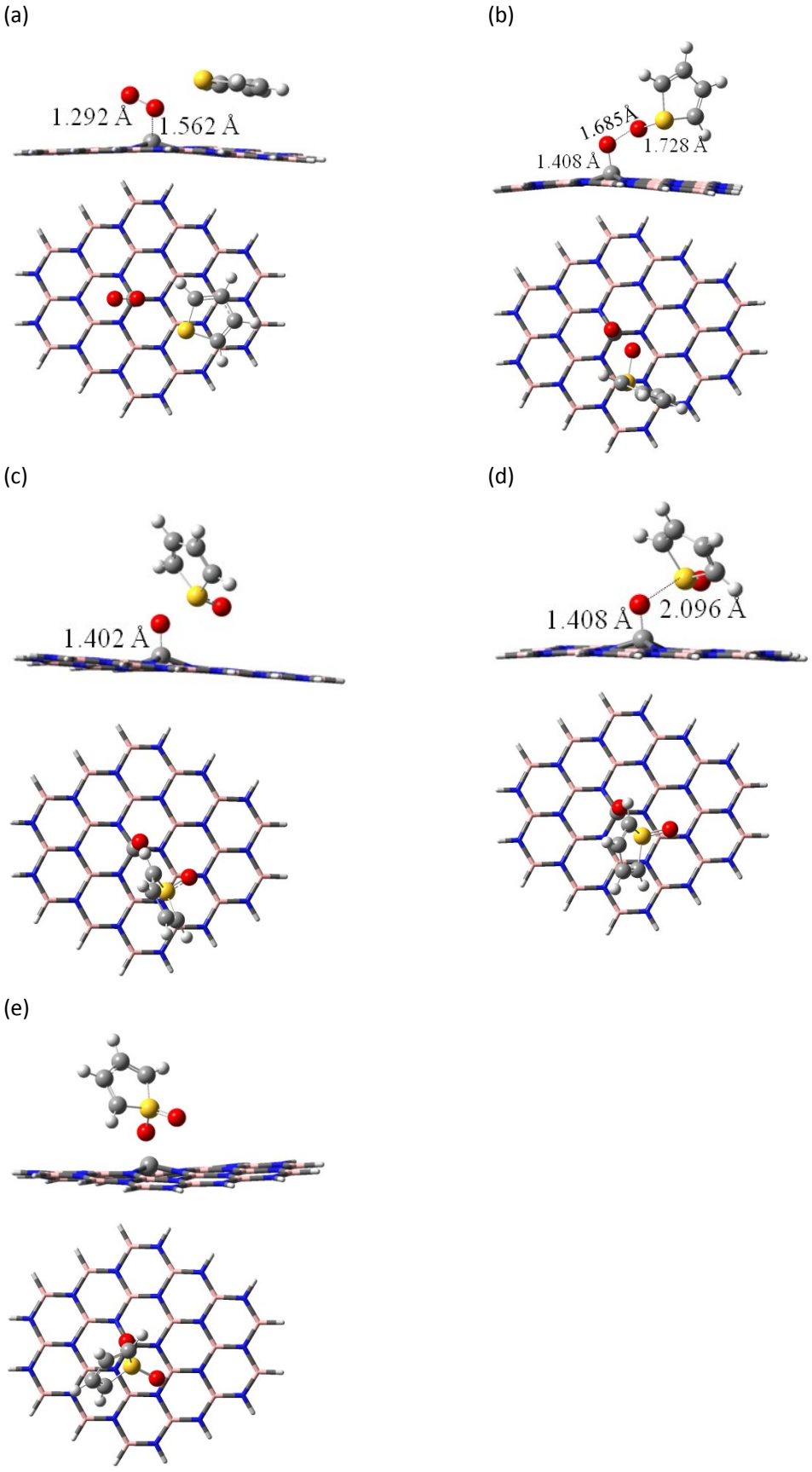

Figure S5 TH oxidation on C_B model. (a) O2 and TH co-adsorption (b)TS1 (c) IM1 (d) TS2 (e) FS

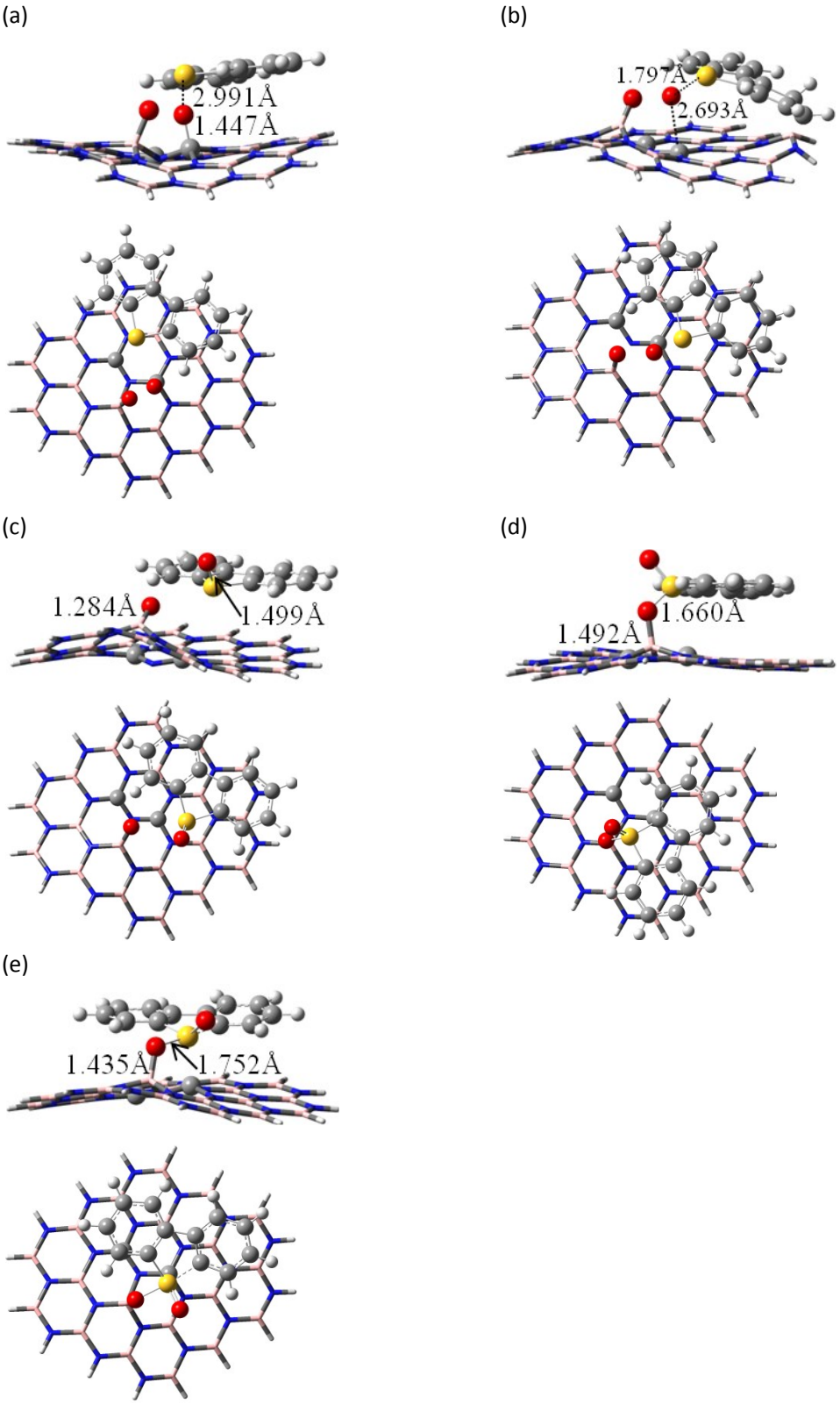

Figure S6 DBT oxidation on C_{2B} model. (a) O_2 and DBT co-adsorption (b)TS1 (c) IM1 (d) TS2 (e) FS

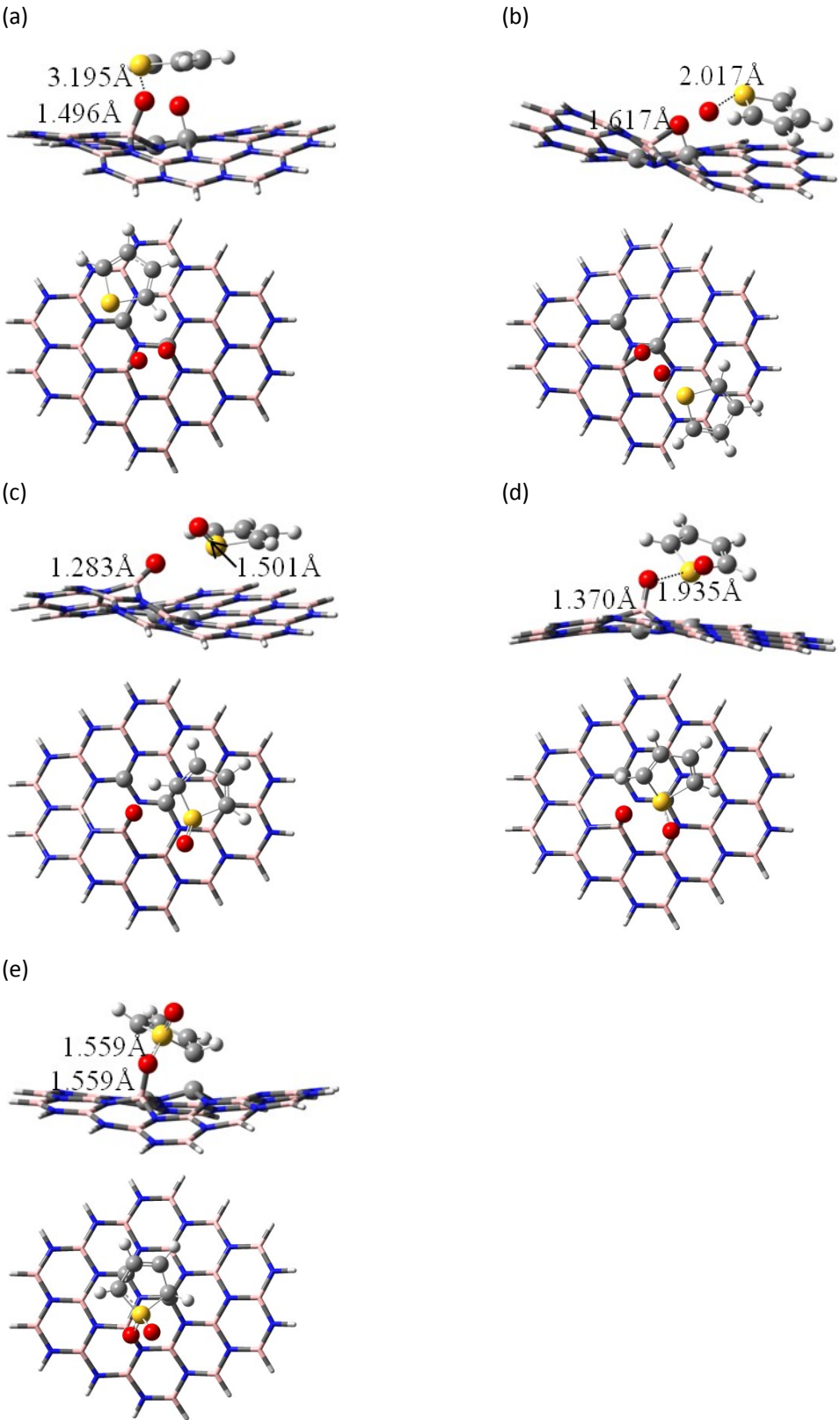

Figure S7 TH oxidation on C_{2B} model. (a) O_2 and TH co-adsorption (b)TS1 (c) IM1 (d) TS2 (e) FS

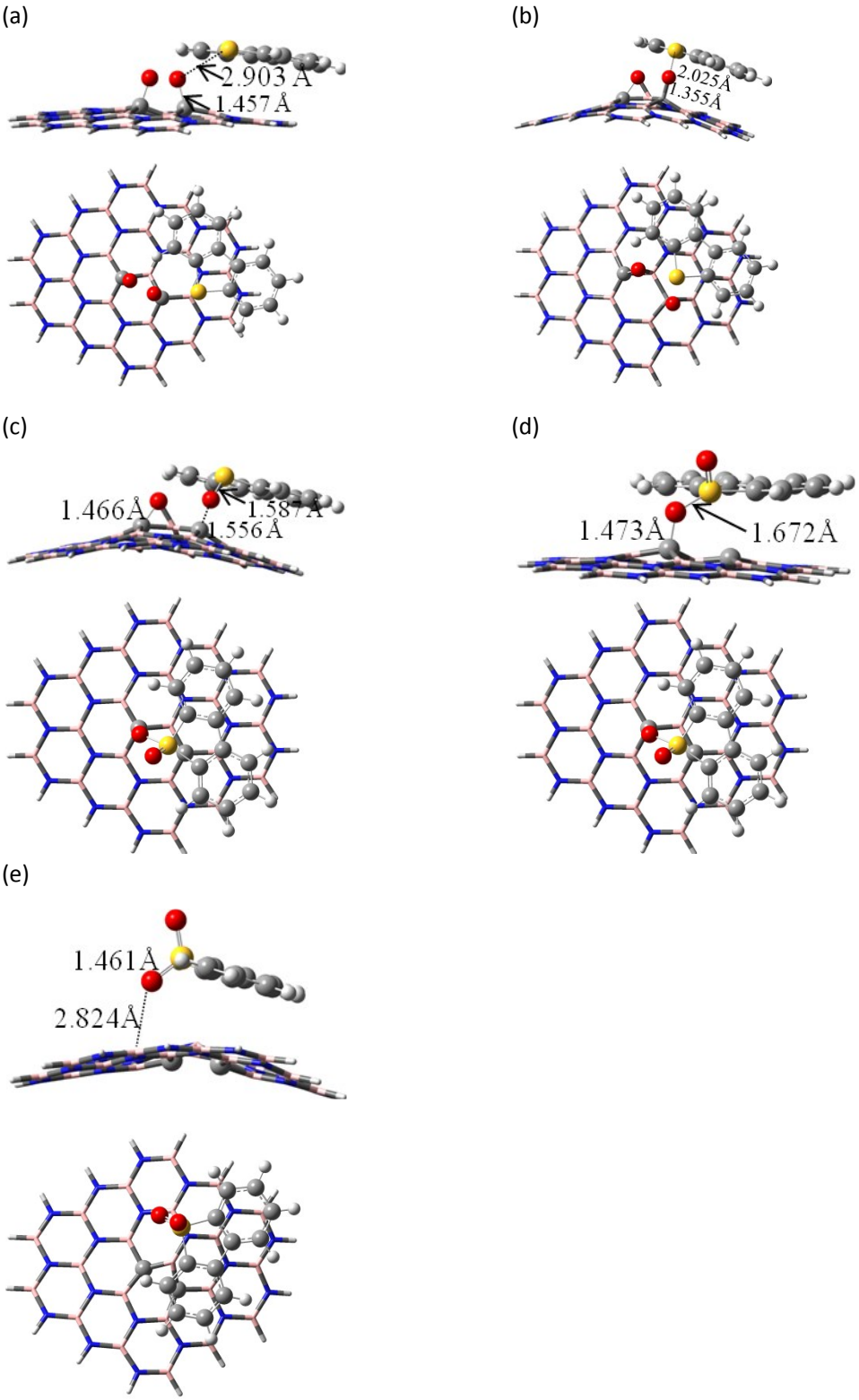

Figure S8 DBT oxidation on C_{2N} model. (a) O_2 and DBT co-adsorption (b)TS1 (c) IM1 (d) TS2 (e) FS

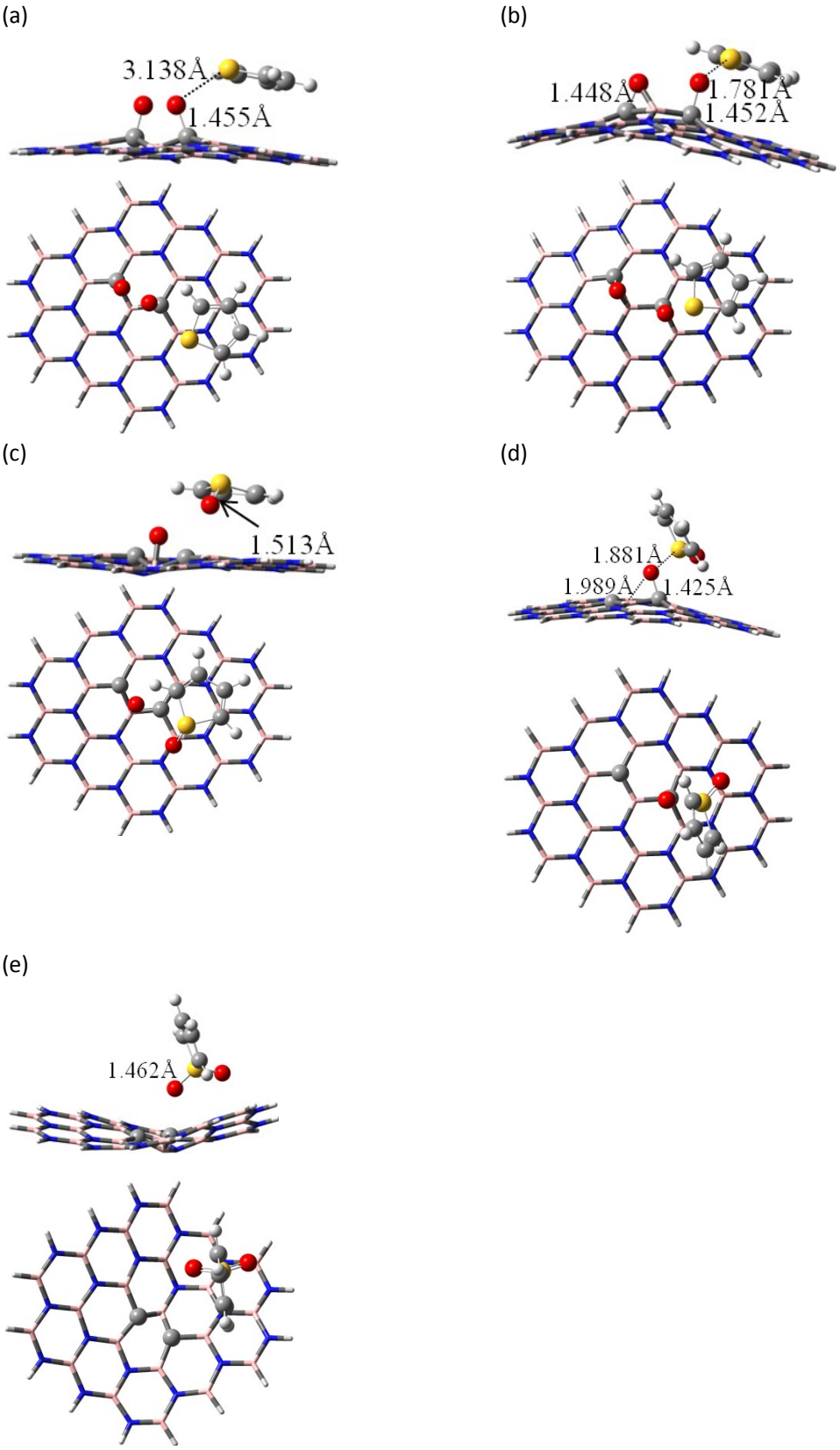

Figure S9 TH oxidation on C_{2N} model. (a) O_2 and TH co-adsorption (b)TS1 (c) IM1 (d) TS2 (e) FS

Table S1 The adsorption Gibbs free energies ($G_{ad,}$ kcal/mol) of thiophene (TH) on C_N monolayer.

	sulfcompound	sulfcompound $+O_2$	TS1	IM1	TS2	FS
TH	3.5	5.2	57.3	14.9	30.5	23.8
DBT	-2.6	1.5	45.6	4.2	29.3	-11.7

Table S2 The adsorption Gibbs free energies ($G_{ad,}$ kcal/mol) of TH and DBT on C_B monolayer.

	Sulfite	sulfite+O_2	TS1	IM1	TS2	FS
TH	3.9	-13.6	43.7	8.5	15.5	6.3
DBT	-0.4	-26.2	30.0	-6.1	4.0	-13.1