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Supplementary Information File

Metals (Al, Fe, Zn) doped in single walled carbon nanotube for catalytic oxidation of H_2O to H_2O_2: A theoretical investigation

Yang Chen, [a] Shuang Zhang, [a] Dan Mao, [a] Rui-Fang Xie, [a] Qiao-Qiao Qin, [a] Xin-Tong Su, [b] Bin Zhai, [c] Lai-Cai Li *[a] and Yan Zheng *[a]

[a] *College of Chemistry and Material Science, Sichuan Normal University, Chengdu 610068, China*

[b] *Chengdu Tongneng Compressed Natural Gas Co., LTD, Chengdu 610037, China*

[c] *Systems Engineering Research Institute of China State Shipbuilding Corporation, Beijing 100094, China*

Email: zhengyanchem@163.com; lilcmail@163.com

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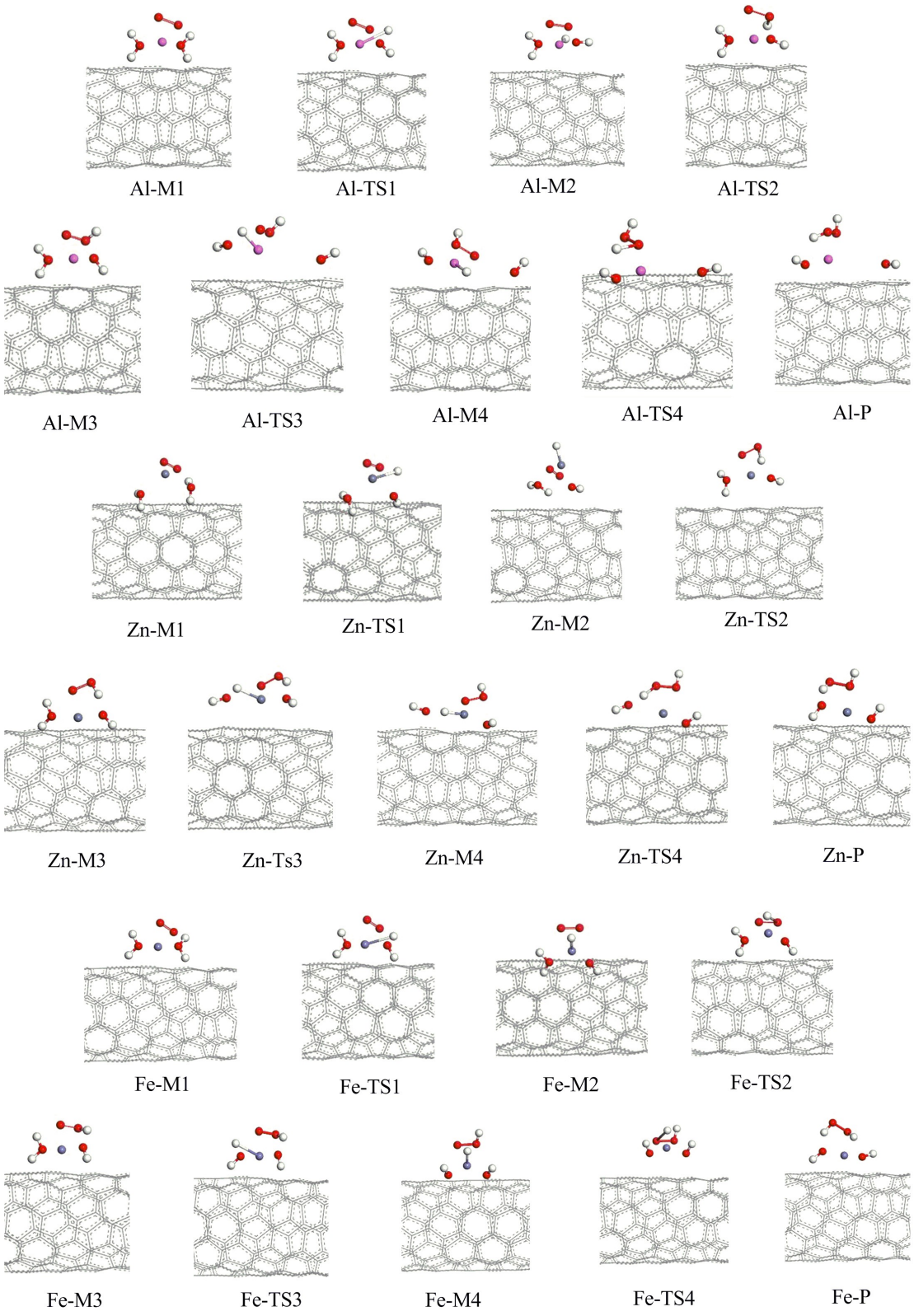


Fig. S1. The optimized configuration diagrams of the reactants, products and each intermediate of the catalytic Path I.

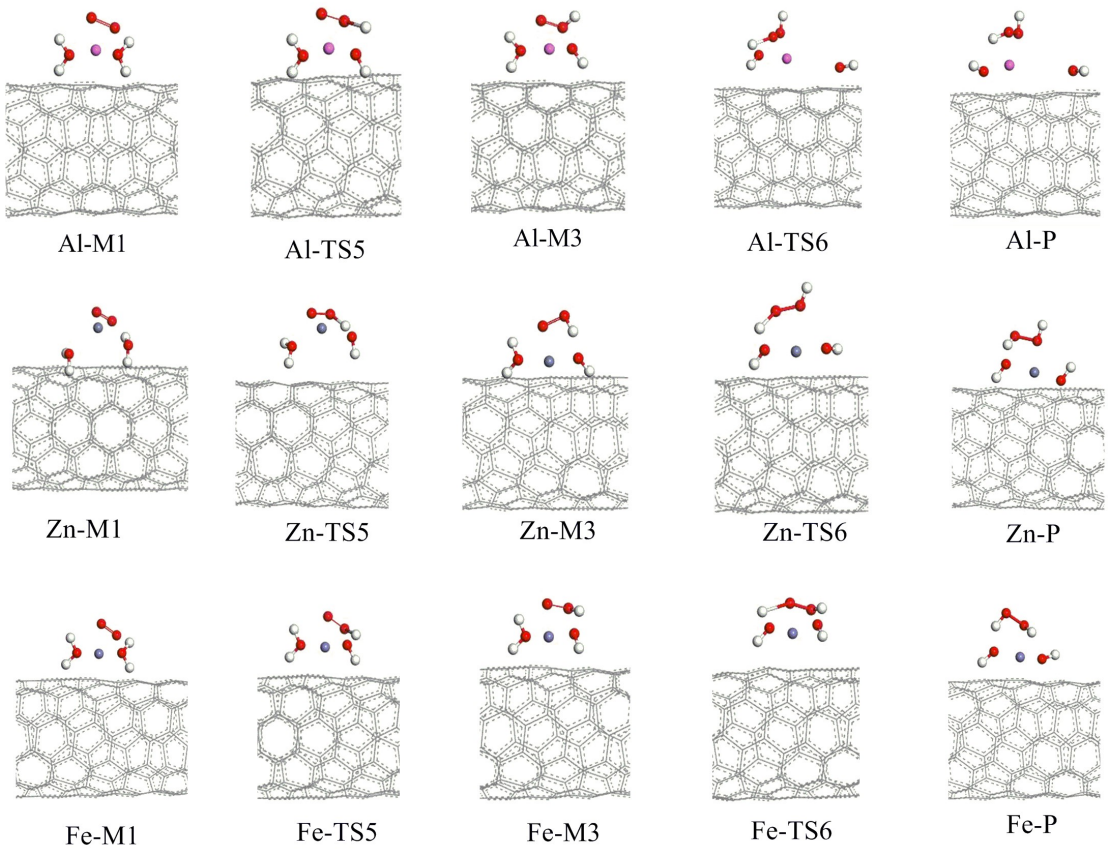


Fig. S2. The optimized configuration diagrams of the reactants, products and each intermediate of the catalytic Path II.

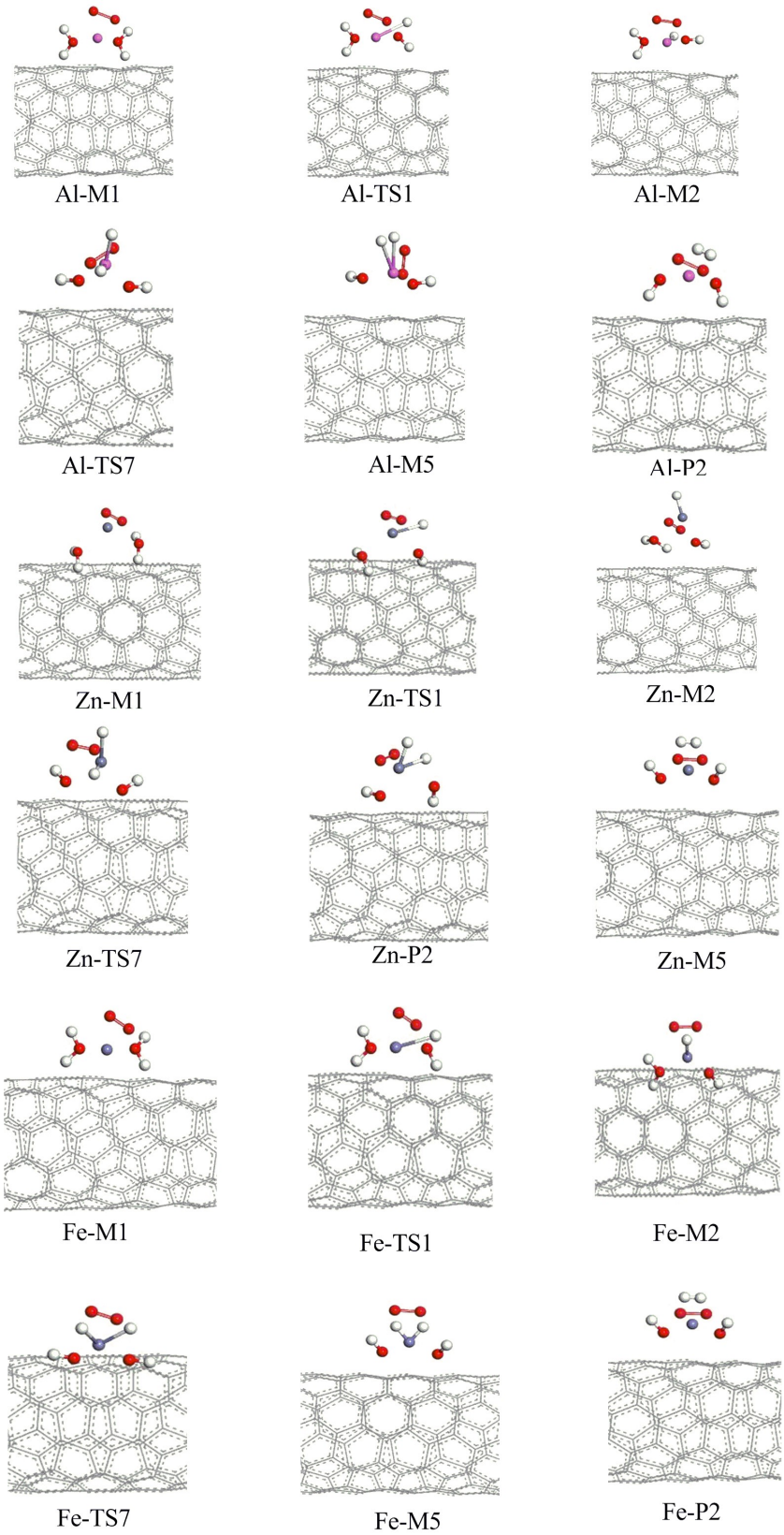


Fig. S3. The optimized configuration diagrams of the reactants, products and each intermediate of the catalytic Path III.

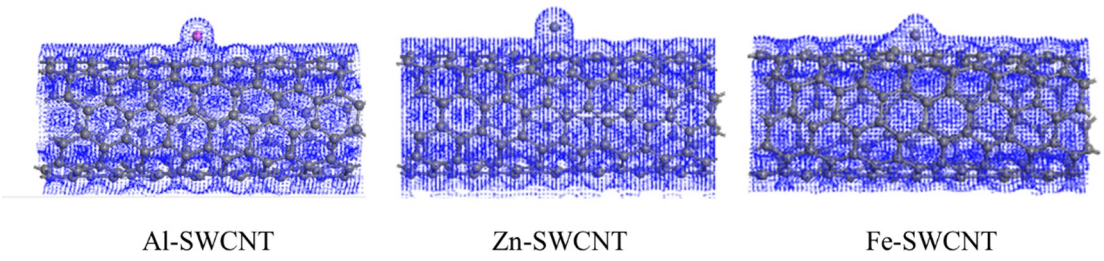


Fig. S4. Electron density diagram of R (Al, Zn, Fe)-SWCNT.

Table S5. Adsorption energy of H_2O and O_2 on three catalysts.

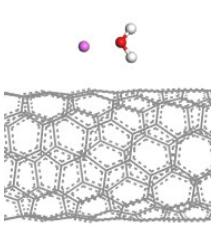
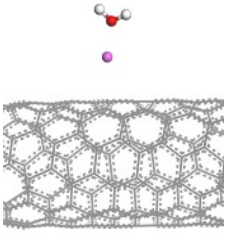
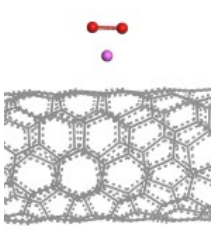
Metal	Al1	Zn1	Fe1	Al2	Zn2	Fe2	Al	Zn	Fe
Position									
E_{ads}(eV)	-0.77	-0.31	-2.15	-0.42	-0.30	-2.02	-1.99	-1.17	-2.59

Table S6. Configuration parameters of each stationary point in the reaction process of Path I.

Metal	Compounds	Bond length（Å）					
		R-H(1)	H(1)-O(1)	H(1)-O(2)	R-H(3)	H(3)-O(4)	H(3)-O(3)
Al	Al-M1	2.524	0.997	2.100	2.419	0.998	—
	Al-TS1	2.226	1.845	—	—	—	—
	Al-M2	1.590	—	2.900	—	—	—
	Al-TS2	2.763	—	1.689	—	—	—
	Al-M3	—	—	—	2.364	0.994	2.505
	Al-TS3	—	—	—	1.731	1.555	—
	Al-M4	—	—	—	1.574	—	2.825
	Al-TS4	—	—	—	1.986	—	1.707
Zn	Zn-M1	2.406	1.020	1.626	2.808	0.977	—
	Zn-TS1	2.025	1.787	—	—	—	—
	Zn-M2	1.513	—	3.394	—	—	—
	Zn-TS2	2.015	—	2.188	—	—	—
	Zn-M3	—	—	—	2.453	0.980	2.330
	Zn-TS3	—	—	—	1.912	0.203	—
	Zn-M4	—	—	—	1.555	—	2.825
	Zn-TS4	—	—	—	1.905	—	2.021
Fe	Fe-M1	2.182	0.997	1.868	2.503	0.977	
	Fe-TS1	1.827	1.572	—	—	—	—
	Fe-M2	1.465	—	2.415	—	—	—
	Fe-TS2	1.880	—	1.697	—	—	—
	Fe-M3	—	—	—	2.450	0.979	2.550
	Fe-TS3	—	—	—	1.955	1.616	—
	Fe-M4	—	—	—	1.483	—	2.413
	Fe-TS4	—	—	—	2.014	—	1.528

Table S7. Activation energy of each reaction step of Path I.

Path	Metal	Compounds	E_r(kcal/mol)	E_a(kcal/mol)
Path I	Al	Al-M1	0.00	
		Al-TS1	35.39	35.39
		Al-M2	-20.35	
		Al-TS2	-15.89	4.47
		Al-M3	-19.96	
		Al-TS3	33.11	53.07
		Al-M4	37.15	
		Al-TS4	126.90	89.74
		Al-P	67.84	
	Fe	Fe-M1	0.00	
		Fe-TS1	72.96	72.96
		Fe-M2	34.26	
		Fe-TS2	84.29	50.03
		Fe-M3	7.98	
		Fe-TS3	103.22	95.24
		Fe-M4	33.50	
		Fe-TS4	112.71	79.22
		Fe-P	16.88	
	Zn	Zn-M1	0.00	
		Zn-TS1	69.64	69.64
		Zn-M2	0.46	
		Zn-TS2	62.70	62.24
		Zn-M3	7.79	
		Zn-TS3	117.98	110.19
		Zn-M4	49.62	
		Zn-TS4	97.64	48.02
		Zn-P	-1.15	

Table S8. Configuration parameters of each stationary point in the reaction process of Path II.

Metal	Compounds	Bond length（Å）					
		R-H(1)	H(1)-O(1)	H(1)-O(2)	R-H(3)	H(3)-O(4)	H(3)-O(3)
Al	Al-M1	2.524	0.997	2.100	2.419	0.998	—
	Al-M3	—	—	—	2.364	0.994	2.505
	Al-TS5	—	1.690	1.680	—	—	—
	Al-TS6	—	—	—	—	1.462	1.469
Zn	Zn-M1	2.406	1.020	1.626	2.808	0.977	—
	Zn-M3	—	—	—	2.453	0.980	2.330
	Zn-TS5	—	1.282	1.386	—	—	—
	Zn-TS6	—	—	—	—	1.306	1.705
Fe	Fe-M1	2.182	0.997	1.868	2.503	0.977	
	Fe-M3	—	—	—	2.450	0.979	2.550
	Fe-TS5	—	1.420	1.400	—	—	—
	Fe-TS6	—	—	—	—	1.291	1.734

Table S9. Activation energy of each reaction step of Path II.

Path	Metal	Compounds	E_r(kcal/mol)	E_a(kcal/mol)
Path II	Al	Al-M1	0.00	
		Al-TS5	30.51	30.51
		Al-M3	-19.96	
		Al-TS6	4.85	24.81
		Al-P	-1.35	
	Fe	Fe-M1	0.00	
		Fe-TS5	18.67	18.67
		Fe-M3	7.98	
		Fe-TS6	69.79	61.81
		Fe-P	16.88	
	Zn	Zn-M1	0.00	
		Zn-TS5	6.62	6.62
		Zn-M3	7.79	
		Zn-TS6	46.00	38.21
		Zn-P	-1.15	

Table S10. Configuration parameters of each stationary point in the reaction process of Path III.

Metal	Compounds	Bond length（Å）					
		R-H(1)	H(1)-O(1)	H(1)-O(2)	R-H(3)	H(3)-O(4)	H(3)-O(3)
Al	Al-M1	2.524	0.997	2.100	2.419	0.998	—
	Al-TS1	2.226	1.845	—	—	—	—
	Al-M2	1.590	—	2.900	—	—	—
	Al-TS7	2.110	1.685	—	2.318	1.280	—
Zn	Zn-M1	2.406	1.020	1.626	2.808	0.977	—
	Zn-TS1	2.025	1.787	—	—	—	—
	Zn-M2	1.513	—	3.394	—	—	—
	Zn-TS7	2.350	2.488	—	2.413	2.067	—
Fe	Fe-M1	2.182	0.997	1.868	2.503	0.977	
	Fe-TS1	1.827	1.572	—	—	—	—
	Fe-M2	1.465	—	2.415	—	—	—
	Fe-TS7	1.912	1.615	—	2.078	1.643	—

Table S11. Activation energy of each reaction step of Path III.

Path	Metal	Compounds	E_r(kcal/mol)	E_a(kcal/mol)
Path III	Al	Al-M1	0.00	
		Al-TS1	35.39	35.39
		Al-M2	-20.35	
		Al-TS7	61.63	81.98
		Al-M5	5.02	
		Al-P2	-21.63	
	Fe	Fe-M1	0.00	
		Fe-TS1	72.96	72.96
		Fe-M2	34.26	
		Fe-TS7	89.72	55.46
		Fe-M5	3.15	
		Fe-P2	-1.13	
	Zn	Zn-M1	0.00	
		Zn-TS1	69.64	69.64
		Zn-M2	0.46	
		Zn-TS7	115.58	115.12
		Zn-M5	28.16	
		Zn-P2	10.01	

Table S12. Activation energy of each reaction step of Path II for (6,4) SWCNT and (6,6) SWCNT.

Path	SWCNT	Compounds	E_r(kcal/mol)	E_a(kcal/mol)
Path II	(6,4)	Al-M1	0.00	
		Al-TS5	30.51	30.51
		Al-M3	-19.96	
		Al-TS6	4.85	24.81
		Al-P	-1.35	
	(6,6)	Al-M1	0.00	
		Al-TS5	60.65	60.65
		Al-M3	33.42	
		Al-TS6	48.36	14.94
		Al-P	35.29	

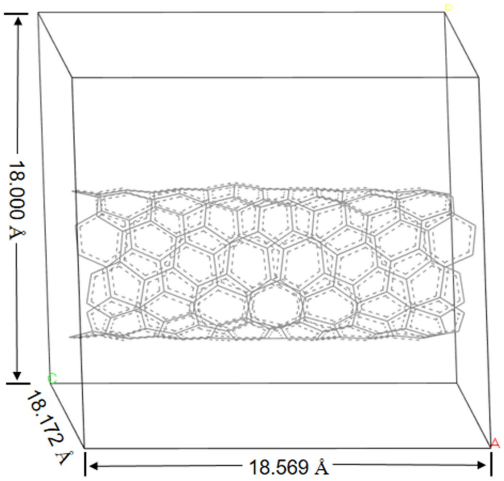


Fig. S13. Diagram of the lattice and the carbon nanotube in it.