Supplementary Information

Agri-waste derived electroactive Carbon-Iron Oxide nanocomposite for Oxygen Reduction Reaction: An experimental and Theoretical study

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Table S1. Comparative ORR performance with recent literature reports.

Active material	Onset potential (V)	n_e	Current density‡ (mA/cm^2)	Tafel slope (mV/dec)	Stability test	Electrolyte	Reference
Fe/N-C	0.81	3.98	-5.4	65.1	5 h	50 mM PBS	[1]
S, N co-doped rGO	0.85	3.8	-3.1	-	10,000 cycles	0.1 M KOH	[2]
N/S-doped CNC/SnO_2	0.68	3.9	-1.0	-	4 h	0.1 M KOH	[3]
CeO_2/biochar carbon	0.79	3.9	-4.4	96	5000 cycles	0.1 M KOH	[4]
Nitrogen-functionalized reduced graphene oxide	0.82	4.1	-3.7	62	-	0.1 M KOH	[5]
Fe Phthalocyanine@ Mesoporous Carbon Nitride	0.62	0.87	-1.2		Shift in onset potential by 20 mV after 3000 cycles	0.1 M $HClO_4$	[6]
Biomass carbon from pine needles	0.96	3.7-3.9	-4.8	62.6	1 h	0.1 M KOH	[7]
TAPX-NDI-COF	-	~3.5	-5.2	84.2-76.4	3 h	0.1 M NaOH	[8]
Fe-BN-C catalysts derived from ZIF-8	0.96	3.5-3.7	-6.1	-	10 h	0.1 M KOH	[9]
Fe-N-C-2	0.96	~3.9	-5.8	74.9	11 h	0.1 M KOH	[10]
Fe_3O_4@FeNC	1.0	3.96	-6.9	58.8	11 h	0.1 M KOH	[11]
FeS/Fe_3C@NS-C-900	-	3.7-4.2	-6.8	94	5.6 h	0.1 M KOH	[12]

Pt/C	0.97	3.70-3.86	-5.7	106.6	11 h	50 mM Fe_{28}	[13]
Fe_3O_4 partially graphitized composite	0.82	3.76-3.94	-7.7	86	40 h	0.1 M KOH	**Present work**

Figure S1: (a,c,e,g) N_2 adsorption-desorption isotherm and (b,d,f,h) pore size distribution curves of CFe-0, CFe-1, CFe-2 and CFe-3.

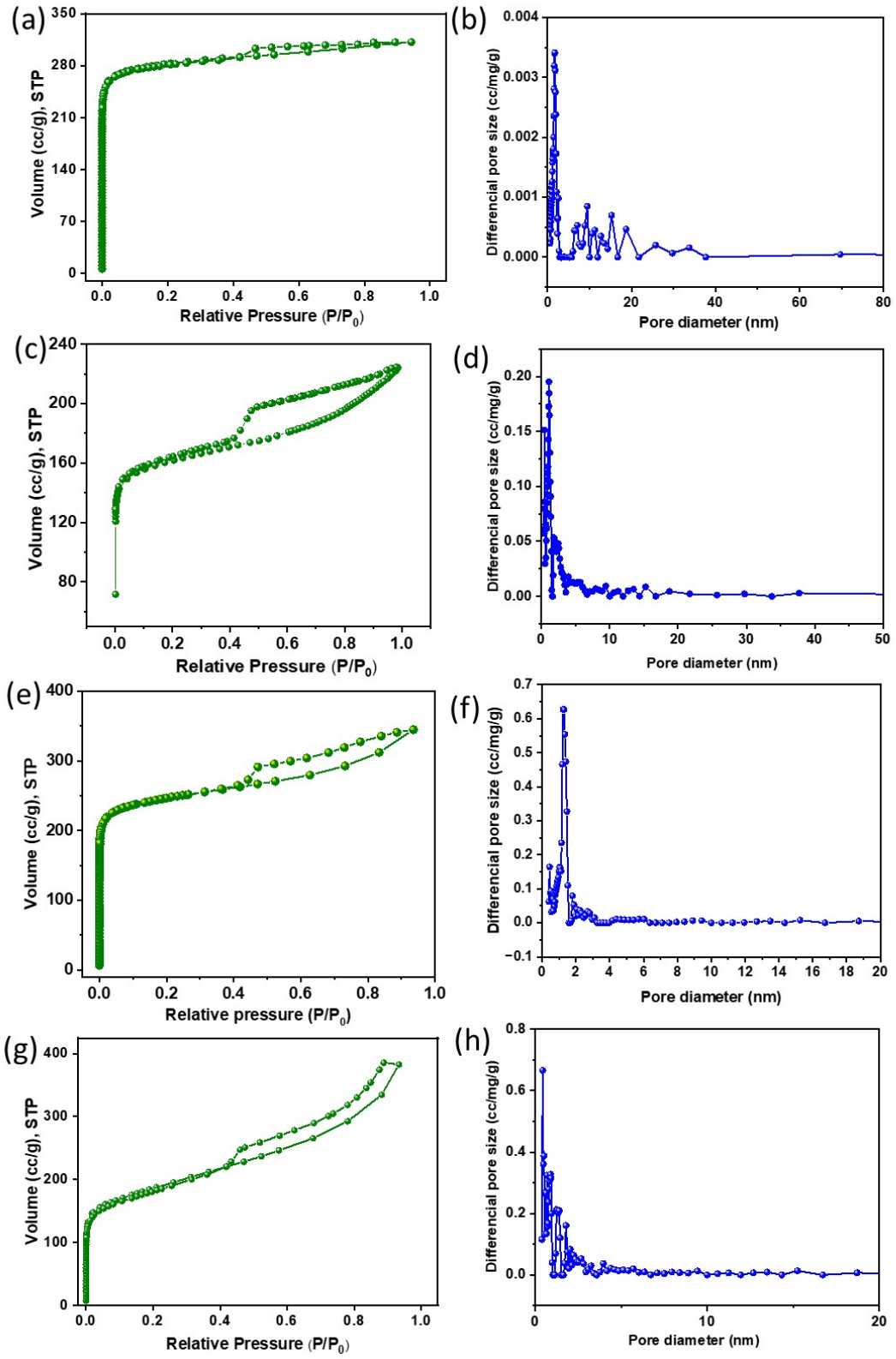
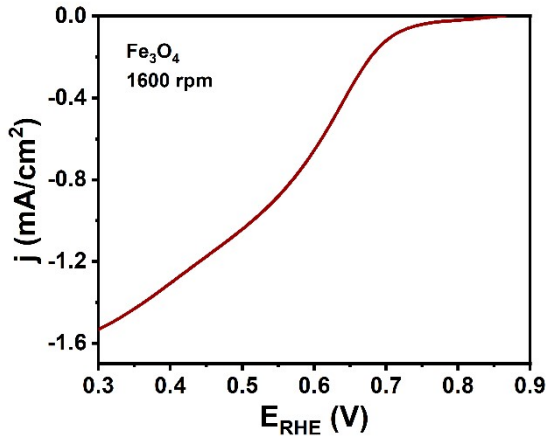


Figure S2. LSV of Fe_3O_4 at 1600 rpm



Theoretical study:

Figure S3 shows the side and top view of the pristine CFe-2 structure. The interlayer distance between the Fe3O4 (022 plane) and graphite in the optimized heterostructure is 3.29 Å, whereas the interlayer distance for graphene sheets is 3.7 Å. Firstly, we considered possible adsorption sites of oxygen molecule on the surface. As illustrated in **Figure S4**, three different favorable binding sites for oxygen are identified: one on the top of tetragonal Fe (S1), the second (S2) and third (S3) are on the edge of differently bonded surface Fe. Compared to other sites, S2 exhibits the lowest adsorption energy, indicating that it is the most thermodynamically stable. In the charge density difference (CDD) figure the yellow-colored electron cloud around adsorbed O atom indicates the accumulation of charge, while the cyan colored electron cloud around active Fe illustrates the loss of electrons.

Figure S3. The side and top view of the optimized pristine CFe-2 structure.

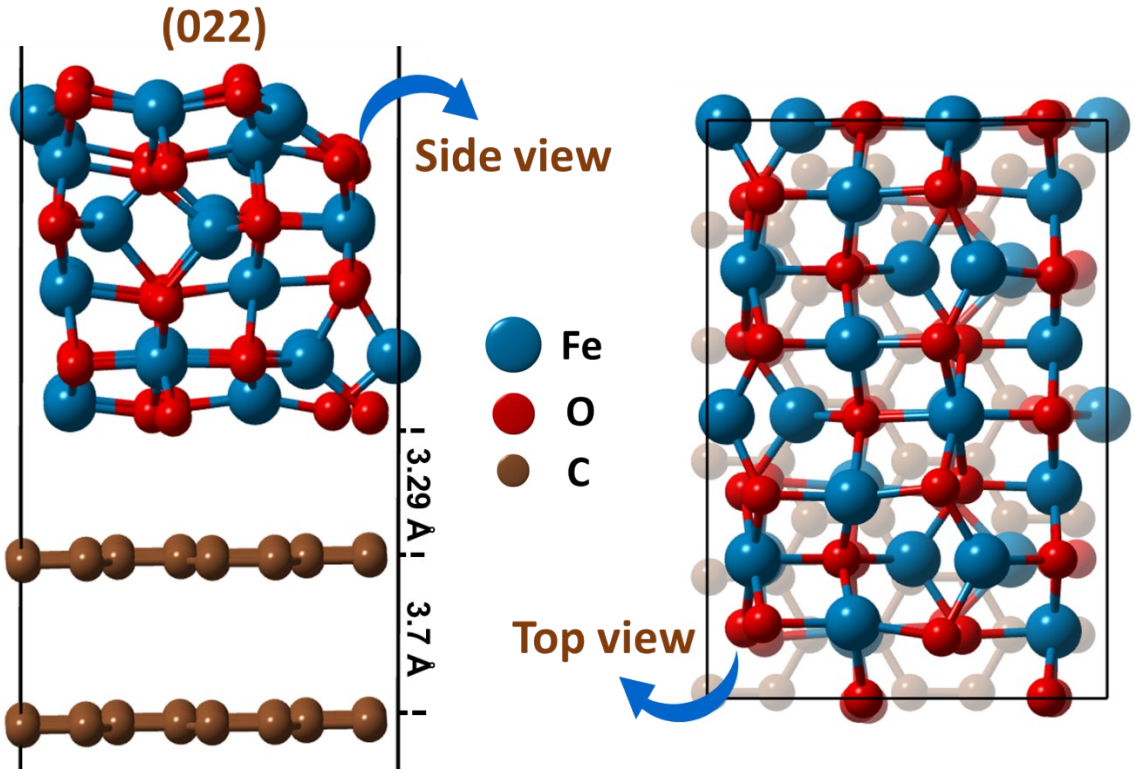


Figure S4. (a) Three different possible O_2 adsorption sites S_1, S_2, and S_3. **(b)** The most stable O_2 adsorbed structure (on S_2 site).

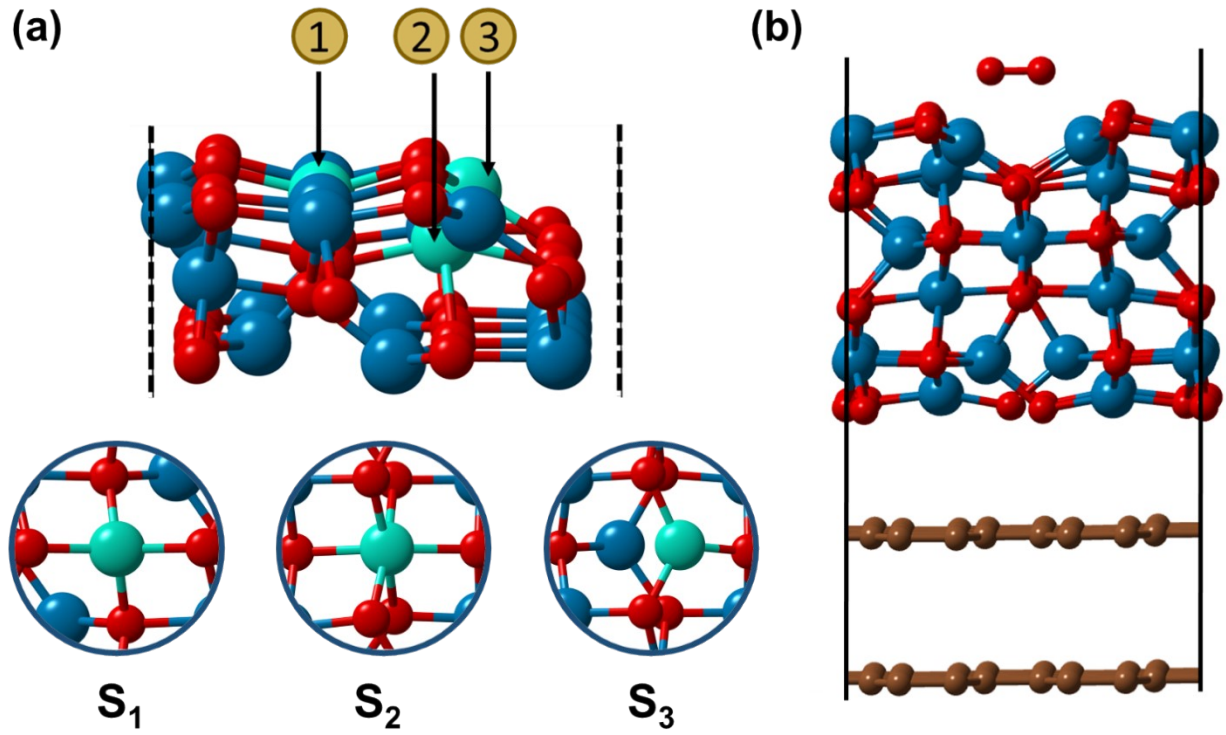


Figure S5: EDS of CFe-2.

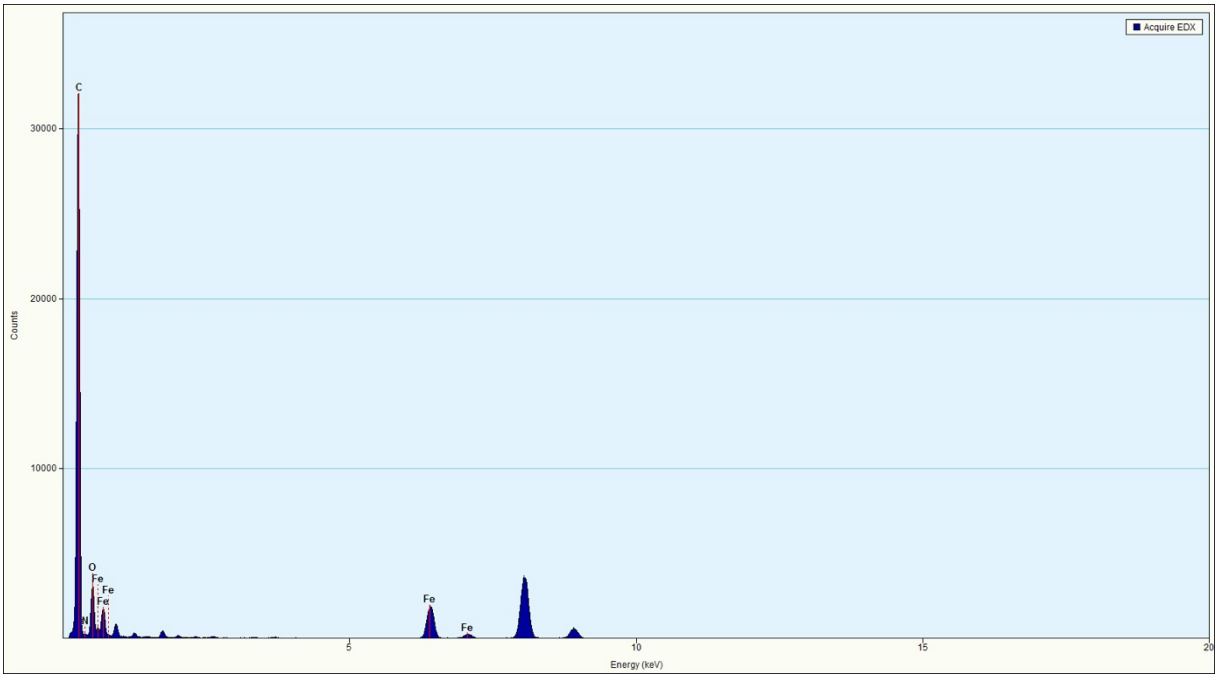


Table S2. EDS, XPS, and CHN analysis.

EDS element quantification (at. %)				
	C (K)	N (K)	O (K)	Fe (K)
CFe-2	93.89	0.42	4.36	1.31
XPS quantification (at. %)				
	C 1s	N 1s	O 1s	Fe 2p
CFe-2	92.34	0.67	5.17	1.82
CHN analysis				
Sample	**C**	**H**	**N**	**others***
CFe-0	52.677	2.127	1.707	43.489
CFe-1	72.001	0.862	1.834	25.303
CFe-2	70.809	1.300	1.810	26.081
CFe-3	61.926	0.580	1.712	35.782

* Contain oxygen and iron content in CFe-1, CFe-2, and CFe-3 and only oxygen for CFe-0.

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