

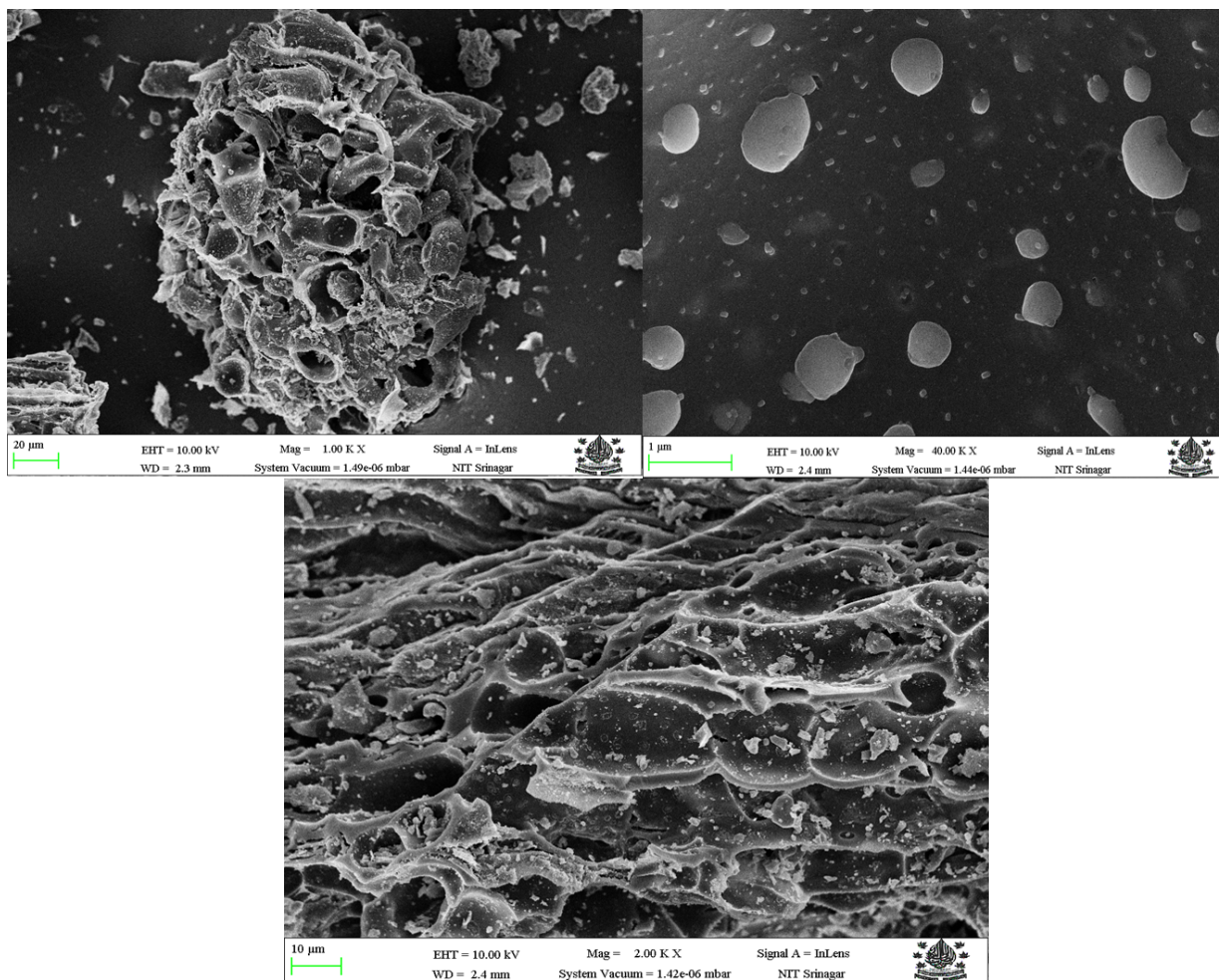
## Supporting Information File

### **Electrochemical analysis of glyphosate using porous biochar surface corrosive nZVI nanoparticles**

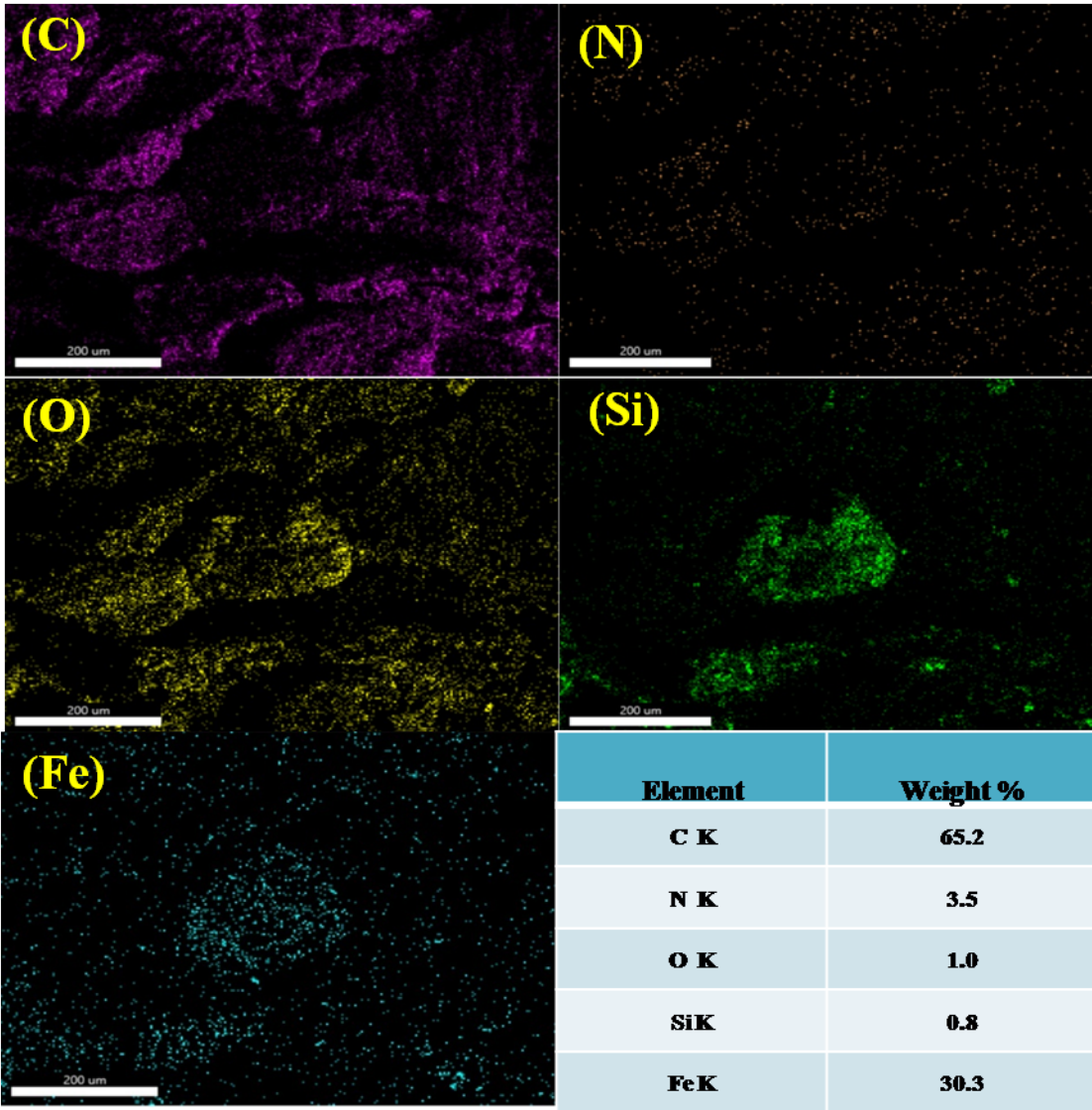
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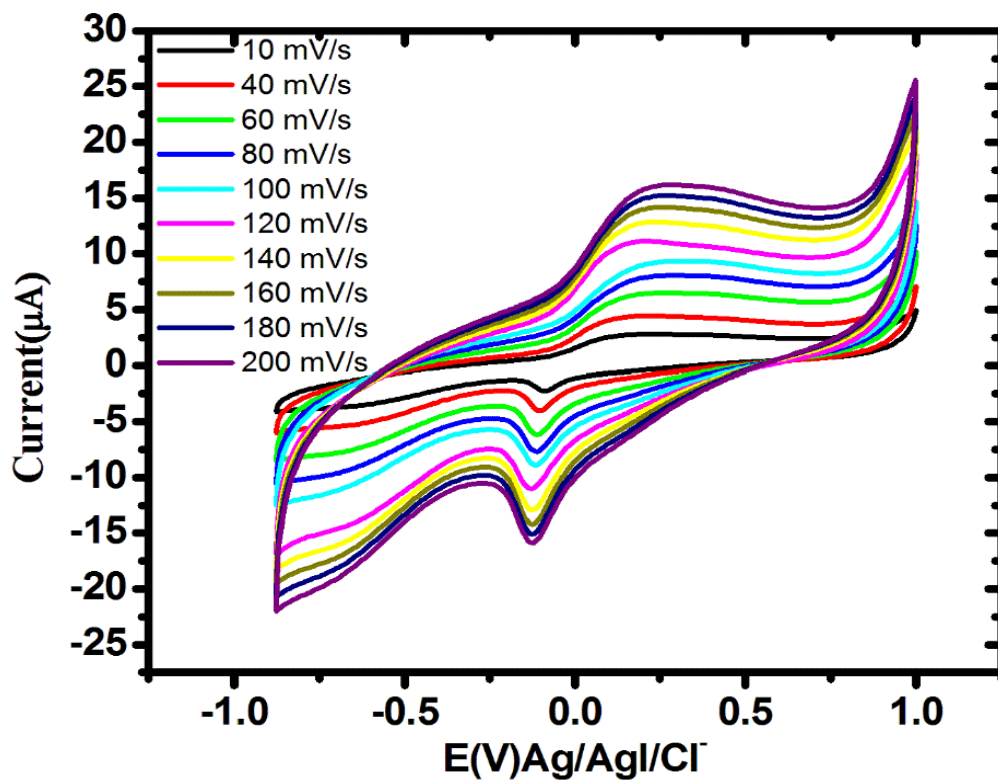
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**Figure S1:** SEM Images of nZVI@Biochar nanocomposite.



**Figure S2:** Elemental analysis of synthesized material with the corresponding weight percentage of different elements.



**Figure S3:** Cyclic voltammogram of fnZVI@Biochar with increase in concentrations of Glyphosate.

**Table T1:** Cartesian coordinates of optimized Geometries

<b>Cartesian Coordinates (Angstroms) of Biochar-Glyphosate</b>					
<b>S.No.</b>	<b>At.No.</b>	<b>Symbol</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
1	6	C	6.293126	0.605730	-0.419871
2	6	C	5.312027	-0.407483	-1.038288
3	6	C	3.078802	-1.282638	-0.942340
4	8	O	7.325320	1.183448	-1.223437
5	8	O	6.186494	0.925279	0.792601
6	8	O	1.656485	-1.475832	1.369009
7	8	O	0.846182	0.412345	-0.268733
8	8	O	0.383933	-2.293791	-0.779376
9	7	N	4.015303	-0.315475	-0.352035
10	15	P	1.473336	-1.168727	-0.092691
11	1	H	0.729339	0.608266	-1.201236
12	1	H	-0.462909	-2.233702	-0.331215
13	1	H	4.137011	-0.519553	0.619325
14	1	H	3.471231	-2.271963	-0.832181
15	1	H	2.948574	-1.064273	-1.981693
16	1	H	5.181801	-0.189116	-2.077643
17	1	H	5.704452	-1.396809	-0.928130
18	1	H	7.028368	1.238603	-2.134688
19	6	C	-1.207512	-1.375197	3.405262
20	6	C	-1.562118	-1.726489	2.091198
21	6	C	-1.736944	-0.728429	1.135357
22	6	C	-1.560371	0.608550	1.484114

23	6	C	-1.208972	0.947468	2.788711
24	6	C	-1.034654	-0.066349	3.746681
25	6	C	-2.088343	-1.067347	-0.169240
26	6	C	-1.735197	1.606610	0.528273
27	6	C	-2.086595	1.267692	-0.776325
28	6	C	-2.263169	-0.069286	-1.125081
29	6	C	-2.261421	2.265753	-1.732165
30	6	C	-2.081147	3.612286	-1.371241
31	6	C	-1.737142	3.944073	-0.094093
32	6	C	-1.558623	2.943589	0.877029
33	6	C	-1.204031	3.276305	2.195923
34	6	C	-1.032884	2.299244	3.131652
35	1	H	-0.762955	2.563119	4.132856
36	1	H	-1.067600	4.302304	2.467241
37	1	H	-1.072420	-2.139317	4.141992
38	1	H	-0.764730	0.190455	4.749723
39	1	H	-2.214640	4.381481	-2.102965
40	1	H	-1.602304	4.972067	0.170380
41	6	C	-1.742392	-3.073022	1.730274
42	6	C	-2.086398	-3.404810	0.453126
43	6	C	-2.264916	-2.404325	-0.517996
44	1	H	-1.608900	-3.842217	2.461998
45	1	H	-2.221235	-4.432804	0.188652
46	6	C	-2.619508	-2.737042	-1.836890
47	6	C	-2.790656	-1.759981	-2.772620
48	6	C	-2.614568	-0.408204	-2.429678

49	1	H	-2.755939	-3.763041	-2.108209
50	1	H	-3.060585	-2.023856	-3.773823
51	6	C	-2.616028	1.914460	-3.046229
52	1	H	-2.751119	2.678580	-3.782959
53	6	C	-2.788886	0.605612	-3.387648
54	1	H	-3.058809	0.348808	-4.390690

**Cartesian Coordinates (Angstroms) of nZVI@Biochar**

S.No.	At.No.	Symbol	X	Y	Z
1	26	Fe	-0.256649	-2.900482	0.340174
2	26	Fe	-2.447969	-2.396479	0.459128
3	26	Fe	-1.600026	-0.141543	0.867490
4	26	Fe	-0.412277	0.873555	-0.921268
5	26	Fe	0.603688	-0.842286	0.315954
6	26	Fe	-1.218481	-1.225205	-1.185844
7	6	C	-1.870411	1.525807	3.124198
8	6	C	-0.614278	0.910795	2.845194
9	6	C	-0.592020	-0.457540	2.456455
10	6	C	-1.814335	-1.190533	2.351501
11	6	C	-3.053394	-0.551790	2.635786
12	6	C	-3.046225	0.820727	3.023245
13	6	C	0.652654	-1.099097	2.170905
14	6	C	-1.791976	-2.565055	1.961004
15	6	C	-0.547302	-3.206613	1.675454

16	6	C	0.675013	-2.473619	1.780408
17	6	C	-0.525043	-4.574947	1.286715
18	6	C	-1.759666	-5.282278	1.190047
19	6	C	-2.956988	-4.665155	1.464726
20	6	C	-3.008774	-3.294824	1.856501
21	6	C	-4.236303	-2.629484	2.147341
22	6	C	-4.257811	-1.307267	2.522977
23	1	H	-5.203432	-0.817972	2.740452
24	1	H	-5.164875	-3.188243	2.067067
25	1	H	-1.885455	2.571067	3.420989
26	1	H	-3.993434	1.307232	3.240063
27	1	H	-1.740706	-6.327392	0.892970
28	1	H	-3.887237	-5.221246	1.385347
29	6	C	0.620344	1.618125	2.941862
30	6	C	1.817667	1.001003	2.667183
31	6	C	1.869452	-0.369329	2.275409
32	1	H	0.601384	2.663239	3.238939
33	1	H	2.747916	1.557093	2.746562
34	6	C	3.096982	-1.034669	1.984569
35	6	C	3.118490	-2.356886	1.608932
36	6	C	1.914072	-3.112362	1.496123
37	1	C	4.025554	-0.475909	2.064842
38	1	C	4.064110	-2.846180	1.391457
39	6	H	0.731089	-5.189959	1.007711
40	1	H	0.746134	-6.235219	0.710921



41	6	C	1.906904	-4.484880	1.108664
42	1	H	2.854113	-4.971385	0.891846

**Cartesian Coordinates (Angstroms) of nZVI@Biochar-Glyphosate**

S.No.	At.No.	SYMBOL	X	Y	Z
1	26	Fe	1.401967	1.600475	-0.561590
2	26	Fe	2.148420	-0.153028	-1.760793
3	26	Fe	1.069799	-1.441533	0.013141
4	26	Fe	-1.291481	-1.240108	0.170010
5	26	Fe	0.070754	0.535103	0.877086
6	26	Fe	-0.189988	-0.068058	-1.423030
7	6	C	2.171017	-3.229228	1.893928
8	6	C	1.730217	-1.940395	2.316488
9	6	C	2.056329	-0.808506	1.518723
10	6	C	2.812792	-0.974822	0.317701
11	6	C	3.239706	-2.272357	-0.080079
12	6	C	2.898694	-3.389241	0.738614
13	6	C	1.627460	0.494842	1.918353
14	6	C	3.140379	0.162185	-0.483671
15	6	C	2.711510	1.465532	-0.084041
16	6	C	1.955047	1.631849	1.116980
17	6	C	3.037623	2.597422	-0.881806
18	6	C	3.793574	2.402433	-2.075319
19	6	C	4.206134	1.148692	-2.459763
20	6	C	3.893448	-0.003313	-1.679321

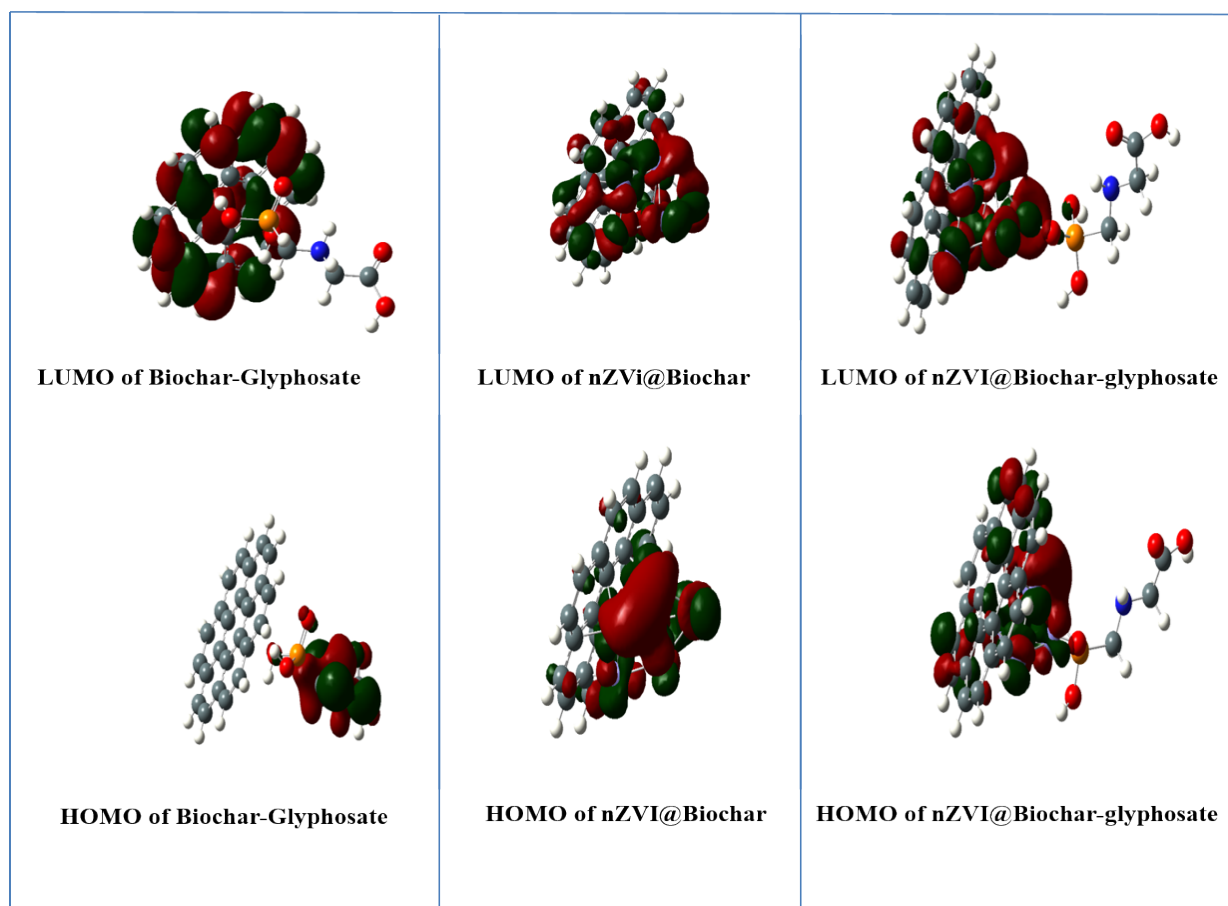
21	6	C	4.308386	-1.315359	-2.054096
22	6	C	3.993264	-2.409099	-1.283218
23	1	H	4.318627	-3.400834	-1.585715
24	1	H	4.883529	-1.440141	-2.967629
25	1	H	1.920979	-4.092643	2.504563
26	1	H	3.225492	-4.379691	0.433467
27	1	H	4.041730	3.268180	-2.683412
28	1	H	4.781412	1.020680	-3.372762
29	6	C	0.974265	-1.745407	3.510000
30	6	C	0.561705	-0.491665	3.894444
31	6	C	0.874391	0.660339	3.114003
32	1	H	0.726109	-2.611154	4.118094
33	1	H	-0.013573	-0.363653	4.807445
34	6	C	0.459454	1.972386	3.488778
35	6	C	0.774575	3.066126	2.717900
36	6	C	1.528133	2.929382	1.514761
37	1	H	-0.115690	2.097168	4.402311
38	1	H	0.449212	4.057860	3.020396
39	6	C	2.596823	3.886255	-0.459246
40	1	H	2.846860	4.749670	-1.069881
41	6	C	1.869145	4.046268	0.696068
42	1	H	1.542347	5.036717	1.001214
43	6	C	-7.156547	1.995355	-0.423687
44	6	C	-7.049029	0.483394	-0.587249
45	6	C	-5.398903	-1.277548	-0.871518
46	8	O	-8.415415	2.477879	-0.261390

47	8	O	-6.220773	2.739291	-0.480527
48	8	O	-2.659829	-0.773590	-1.066295
49	8	O	-3.497615	-1.955726	1.050186
50	8	O	-3.635972	-3.229054	-1.166251
51	7	N	-5.695988	0.037359	-0.334594
52	15	P	-3.659457	-1.730266	-0.546113
53	1	H	-3.920831	-2.752911	1.389841
54	1	H	-2.774590	-3.478696	-1.541491
55	1	H	-5.031687	0.740290	-0.647590
56	1	H	-5.540455	-1.366228	-1.962626
57	1	H	-6.043634	-2.029904	-0.403729
58	1	H	-7.745110	-0.018440	0.097660
59	1	H	-7.399954	0.260425	-1.614195
60	1	H	-9.053999	1.758128	-0.185704

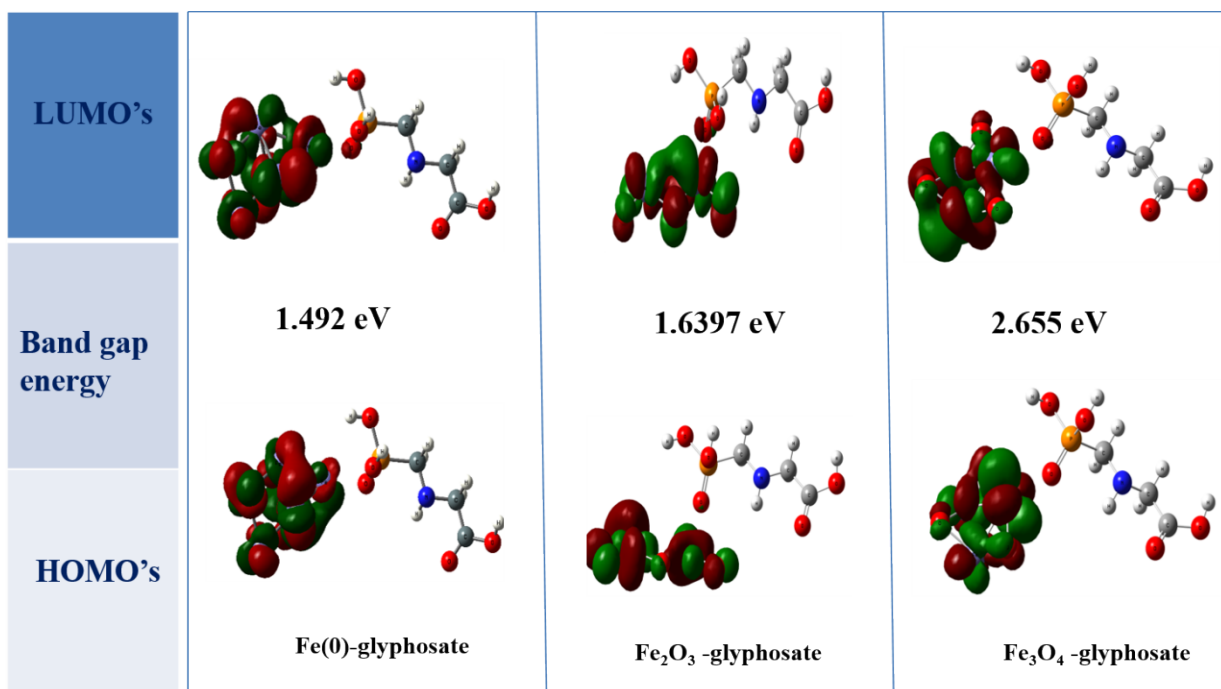
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**Table T2:** Band gap energy values of prepared materials

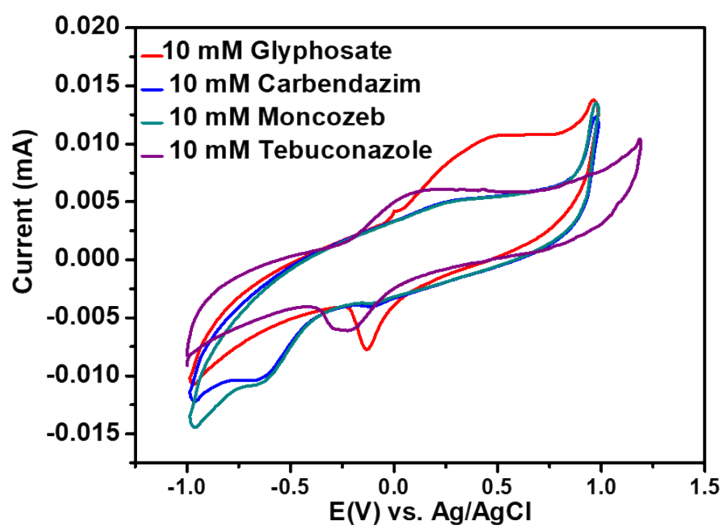
Molecules	HOMO	LUMO	H-L GAP
Biochar-Glyphosate	-5.51 eV	-1.36 eV	4.15 eV
nZVI@Biochar	-3.44 eV	-2.05 eV	1.39 eV
nZVI@Biochar-glyphosate	-3.61 eV	-1.99 eV	1.62 eV



**Figure S4:** Various orientations of HOMO-LUMO for the prepared materials.



**Figure S5:** Band gap energy values of Fe(0), Fe<sub>2</sub>O<sub>3</sub> and Fe<sub>3</sub>O<sub>4</sub> with glyphosate.



**Figure S6:** Cyclic voltammograms of nZVI@Biochar 0.1M KNO<sub>3</sub> with 10 mM concentration of different molecules.