Supporting information

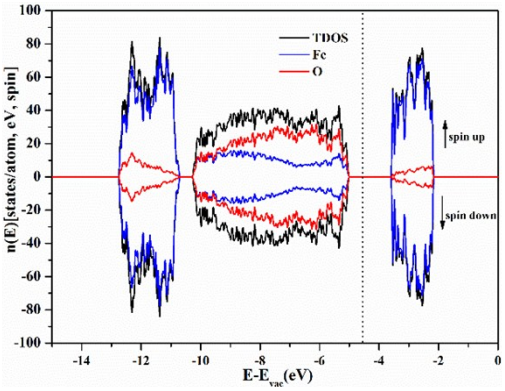
First-principles studies on α-Fe_2O_3 surface slabs and mechanistic elucidation of g-C_3N_4/α-Fe_2O_3 heterojunctions

Sateesh Bandaru[a,b,c,*], Govindarajan Saranya[c], Wei Wei Liu[a] and Niall J English[b,*]

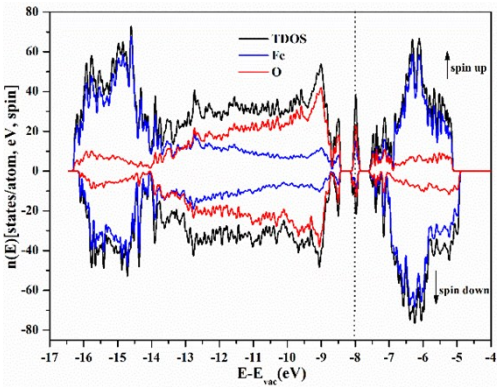
[a] College of Materials and Environmental Engineering, Institute for Advanced Magnetic Materials, Hangzhou Dianzi University, Hangzhou 310018, China.

[b] School of Chemical and Bioprocess Engineering, University College Dublin, Belfield, Dublin 4, Ireland.
[c]Beijing Computational Science Research Center, Beijing 100084, China

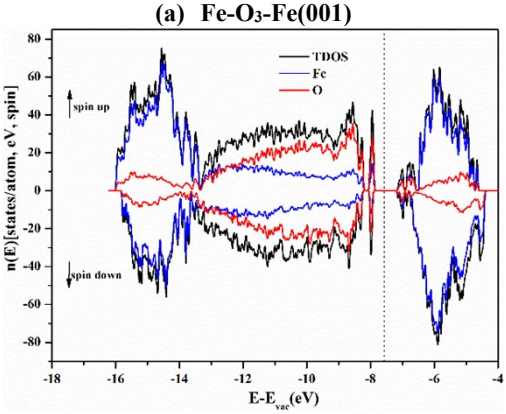
*Corresponding authors: Fax +353-17161177, Tel: +353-1-7161646 (NE), E-Mail: Email: sbandaru@hdu.edu.cn, niall.english@ucd.ie



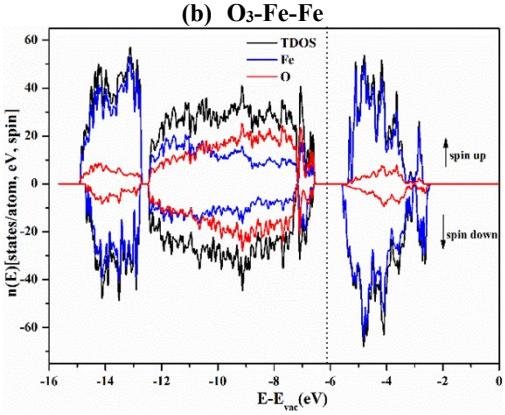
(a) Fe-O_3-Fe(001)



(b) O_3-Fe-Fe



(c) O_2-Fe-Fe



(d) O-Fe-Fe

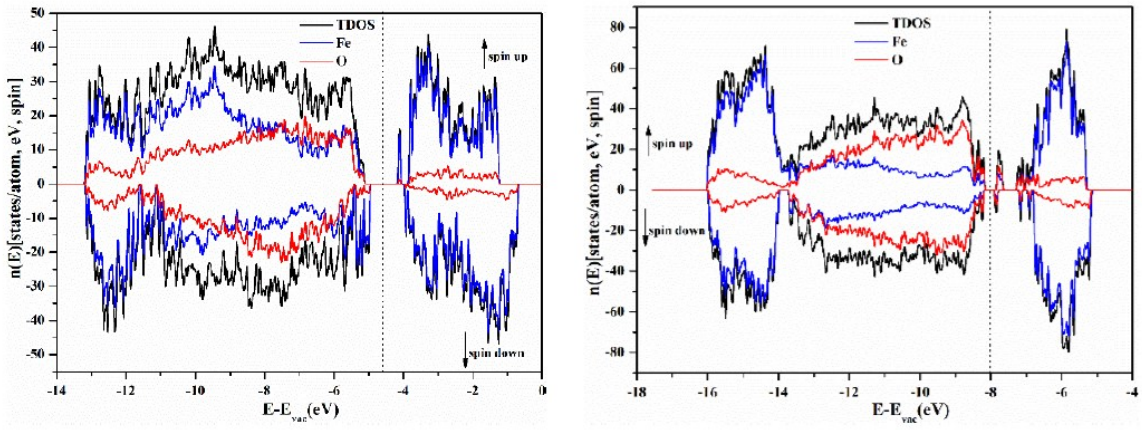


Fig. S1: Vacuum-aligned TDOS and PDOS of Fe and O in (a) to (f) all these surface slabs considered for the study. (Dotted lines indicates a Fermi level)

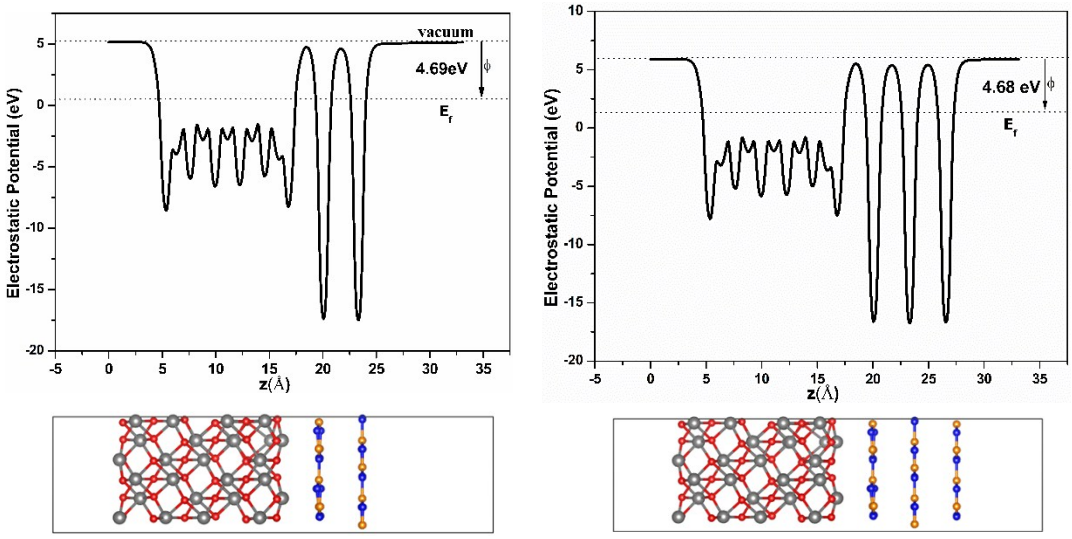


Fig. S2: The electrostatic potential for the *bi*- g-C_3N_4/Fe_2O_3 and tri-g-C_3N_4/Fe_2O_3 heterostructures; work functions(φ) are given in eV.

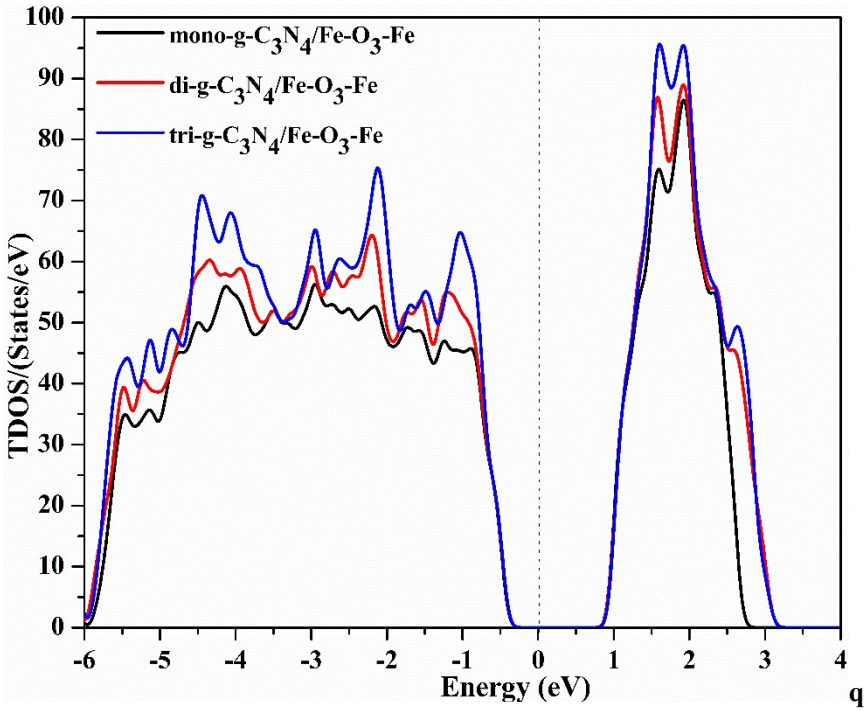


Fig. S3: All three heterostructures (-*mono*, -*bi* and -*tri*-g-C_3N_4/Fe_2O_3) and corresponding Total Density of States, and Fermi level set to zero.

Table S1: Bader charges were computed for the individual monomers Fe-O_3-Fe(001) and g-C_3N_4(001) and the corresponding hetero structure g-C_3N_4/Fe-O_3-F, the charge difference also provide after formation of heterojunction. (Atoms numbered based on POSCAR)

Atom	Monomer	Hetero Structure	Charge Difference
Fe1	1.648965	1.729704	0.080739
Fe2	1.648749	1.845014	0.196265
Fe3	1.75575	1.564501	-0.191249
Fe4	1.820875	1.57111	-0.249765
Fe5	1.639254	1.638005	-0.001249
Fe6	1.513121	1.662747	0.149626
Fe7	1.774883	1.644596	-0.130287
Fe8	1.807786	1.606367	-0.201419
Fe9	1.617467	1.82644	0.208973
Fe10	1.513731	1.773307	0.259576
Fe11	1.76906	1.725422	-0.043638
Fe12	1.774938	1.735746	-0.039192
Fe13	1.656169	1.729624	0.073455
Fe14	1.556404	1.84516	0.288756
Fe15	1.766675	1.564267	-0.202408
Fe16	1.825867	1.570914	-0.254953
Fe17	1.698229	1.637259	-0.06097
Fe18	1.46164	1.663048	0.201408

Fe19	1.769525	1.645005	-0.12452
Fe20	1.757372	1.60613	-0.151242
Fe21	1.503127	1.826573	0.323446
Fe22	1.392702	1.772992	0.38029
Fe23	1.950816	1.726483	-0.224333
Fe24	1.672693	1.735492	0.062799
Fe25	1.648944	1.730052	0.081108
Fe26	1.532329	1.845221	0.312892
Fe27	1.632546	1.564179	-0.068367
Fe28	1.63377	1.571223	-0.062547
Fe29	1.754627	1.63755	-0.117077
Fe30	1.539621	1.662848	0.123227
Fe31	1.738902	1.645374	-0.093528
Fe32	1.811805	1.606058	-0.205747
Fe33	1.584887	1.826267	0.24138
Fe34	1.268532	1.772183	0.503651
Fe35	1.434557	1.725394	0.290837
Fe36	1.680687	1.736063	0.055376
Fe37	1.654838	1.730287	0.075449
Fe38	1.57447	1.845006	0.270536
Fe39	1.700402	1.564026	-0.136376
Fe40	1.594216	1.571275	-0.022941
Fe41	1.570667	1.637985	0.067318
Fe42	1.359983	1.662124	0.302141
Fe43	1.733814	1.64495	-0.088864
Fe44	1.789313	1.606155	-0.183158
Fe45	1.587845	1.826573	0.238728
Fe46	1.434307	1.773311	0.339004
Fe47	1.76473	1.725849	-0.038881
Fe48	0.867043	1.735759	0.868716
O1	-1.130385	-1.062481	0.067904
O2	-1.064953	-1.193469	-0.128516
O3	-0.816725	-1.091822	-0.275097
O4	-1.205796	-1.135041	0.070755
O5	-1.098538	-1.021051	0.077487
O6	-1.125737	-1.186443	-0.060706
O7	-1.20786	-1.188485	0.019375
O8	-1.090957	-1.075855	0.015102
O9	-1.129431	-1.126412	0.003019
O10	-1.084201	-1.132854	-0.048653
O11	-1.12426	-1.119014	0.005246
O12	-0.974422	-1.154721	-0.180299
O13	-1.227662	-1.123819	0.103843

O14	-1.066643	-1.092197	-0.025554
O15	-1.067261	-1.129058	-0.061797
O16	-1.12349	-1.115748	0.007742
O17	-1.150472	-1.174058	-0.023586
O18	-1.015168	-1.148158	-0.13299
O19	-1.112367	-1.062357	0.05001
O20	-1.080855	-1.193775	-0.11292
O21	-0.966529	-1.092295	-0.125766
O22	-1.122057	-1.134371	-0.012314
O23	-1.082272	-1.021164	0.061108
O24	-1.101086	-1.186421	-0.085335
O25	-1.20531	-1.188195	0.017115
O26	-1.027002	-1.075807	-0.048805
O27	-0.975194	-1.126428	-0.151234
O28	-1.150675	-1.132133	0.018542
O29	-1.120443	-1.118759	0.001684
O30	-0.95121	-1.154241	-0.203031
O31	-1.184224	-1.123599	0.060625
O32	-1.162933	-1.092392	0.070541
O33	-1.229813	-1.129132	0.100681
O34	-1.129858	-1.116101	0.013757
O35	-1.152197	-1.173269	-0.021072
O36	-0.957131	-1.148157	-0.191026
O37	-1.11612	-1.062477	0.053643
O38	-1.011904	-1.192122	-0.180218
O39	-0.923698	-1.091663	-0.167965
O40	-1.087889	-1.134377	-0.046488
O41	-1.104901	-1.021662	0.083239
O42	-1.06391	-1.186072	-0.122162
O43	-1.168093	-1.187951	-0.019858
O44	-1.10676	-1.075906	0.030854
O45	-0.997754	-1.12638	-0.128626
O46	-1.097139	-1.131084	-0.033945
O47	-1.125062	-1.118751	0.006311
O48	-0.927507	-1.153918	-0.226411
O49	-1.241591	-1.124145	0.117446
O50	-1.152806	-1.092952	0.059854
O51	-1.01228	-1.128568	-0.116288
O52	-1.076245	-1.115865	-0.03962
O53	-1.156553	-1.173917	-0.017364
O54	-0.948159	-1.147667	-0.199508
O55	-1.091908	-1.062279	0.029629
O56	-0.996849	-1.193818	-0.196969

O57	-1.065564	-1.09213	-0.026566
O58	-0.958028	-1.135122	-0.177094
O59	-1.108932	-1.021644	0.087288
O60	-1.042969	-1.186412	-0.143443
O61	-1.15952	-1.188423	-0.028903
O62	-1.092559	-1.075893	0.016666
O63	-0.930527	-1.1263	-0.195773
O64	-1.134019	-1.13167	0.002349
O65	-1.129315	-1.118711	0.010604
O66	-0.947658	-1.153925	-0.206267
O67	-1.189975	-1.124227	0.065748
O68	-1.065354	-1.093107	-0.027753
O69	-1.034645	-1.129078	-0.094433
O70	-1.19782	-1.115945	0.081875
O71	-1.161857	-1.174094	-0.012237
O72	-1.012689	-1.148063	-0.135374
N1	-0.752446	-0.198962	0.553484
N2	-0.608905	-0.220368	0.388537
N3	-0.673374	-0.221498	0.451876
N4	-0.58232	-0.181627	0.400693
N5	-0.631829	-0.198962	0.432867
N6	-0.538571	-0.220368	0.318203
N7	-0.76247	-0.221498	0.540972
N8	-0.543317	-0.181627	0.36169
N9	-0.73644	-0.198962	0.537478
N10	-0.590026	-0.220368	0.369658
N11	-0.579546	-0.221498	0.358048
N12	-0.509514	-0.181627	0.327887
N13	-0.678501	-0.198962	0.479539
N14	-0.620856	-0.220368	0.400488
N15	-0.598145	-0.221498	0.376647
N16	-0.518876	-0.181627	0.337249
C1	0.833251	0.272573	-0.560678
C2	0.868701	0.274941	-0.59376
C3	0.84434	0.274941	-0.569399
C4	0.817741	0.272573	-0.545168
C5	0.863233	0.274941	-0.588292
C6	1.007075	0.274941	-0.732134
C7	0.771422	0.272573	-0.498849
C8	0.775706	0.274941	-0.500765
C9	0.81264	0.274941	-0.537699
C10	0.772749	0.272573	-0.500176
C11	0.802254	0.274941	-0.527313

C12	0.927574	0.274941	-0.652633