Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Systematic exploration of N, C configurational effects on the ORR performance of Fe-N doped graphene catalysts based on DFT calculations

Guangqi Zhu[1], Fan Liu[1], Dongzi Yang[1], Dong Jia[1], Fengmin Jin[1*], Wei Wang[1*]

[1] School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, China

Table S1. Adsorption energy of oxygen (eV) on Fe-N-C-gra and O-O and Fe-O bond lengths(Å).

Defect	E_{ad}		d_{O-O}		d_{Fe-O}		
	end on	side on	end on	side on	end on	side on	Δ
Fe-3C	--	-1.82	--	1.413	--	1.849 1.851	0.002
Fe-1N	--	-2.28	--	1.424	--	1.841 1.872	0.031
Fe-2N	--	-2.53	--	1.440	--	1.912 1.794	0.118
Fe-3N	-2.08	-2.90	1.354	1.430	1.732	1.838 1.880	0.042
Fe-4C	-1.32	-1.86	1.303	1.408	1.701	1.848 1.852	0.004
Fe-1N-3C	-1.57	-2.17	1.302	1.413	1.691	1.835 1.871	0.036
Fe-2N-2C-oppo	-1.91	-1.98	1.318	1.362	1.710	1.896 1.898	0.002
Fe-2N-2C-pen	-1.30	-1.24	1.299	1.429	1.690	1.842 1.864	0.022
Fe-2N-2C-hex	-1.48	-1.31	1.301	1.416	1.690	1.817 1.918	0.101
Fe-3N-1C	-1.32	-1.30	1.312	1.373	1.730	1.884 1.905	0.021
Fe-4N	-1.33	-1.10	1.315	1.386	1.770	1.900 1.897	0.003

Note: Δ is the difference between the bond lengths of Fe-O_1 and Fe-O_2 (Å).

-- no stable chemical adsorption configuration

Table S2. Adsorption free energy of *OOH, *OH, and *O on Fe-N-C-gra (eV).

Defect	ΔG_{*OOH}	ΔG_{*OH}	ΔG_{*O}
Fe-2N-2C-oppo	2.76	-0.30	0.50
Fe-2N-2C-pen	3.65	0.63	1.20
Fe-2N-2C-hex	3.63	0.57	1.19

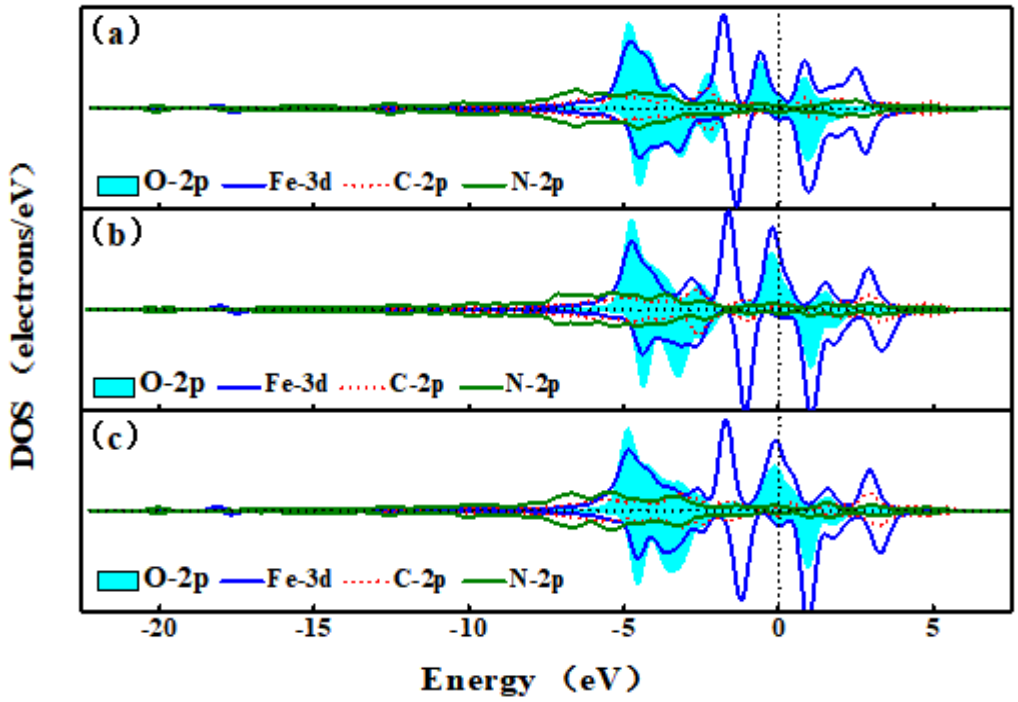

Figure S1. The DOS of the adsorbed O atoms on the Fe-2N-2C-gra in double vacancy (a) O on Fe-2N-2C-oppo site, (b) O on Fe-2N-2C-pen site, (c) O on Fe-2N-2C-hex site.

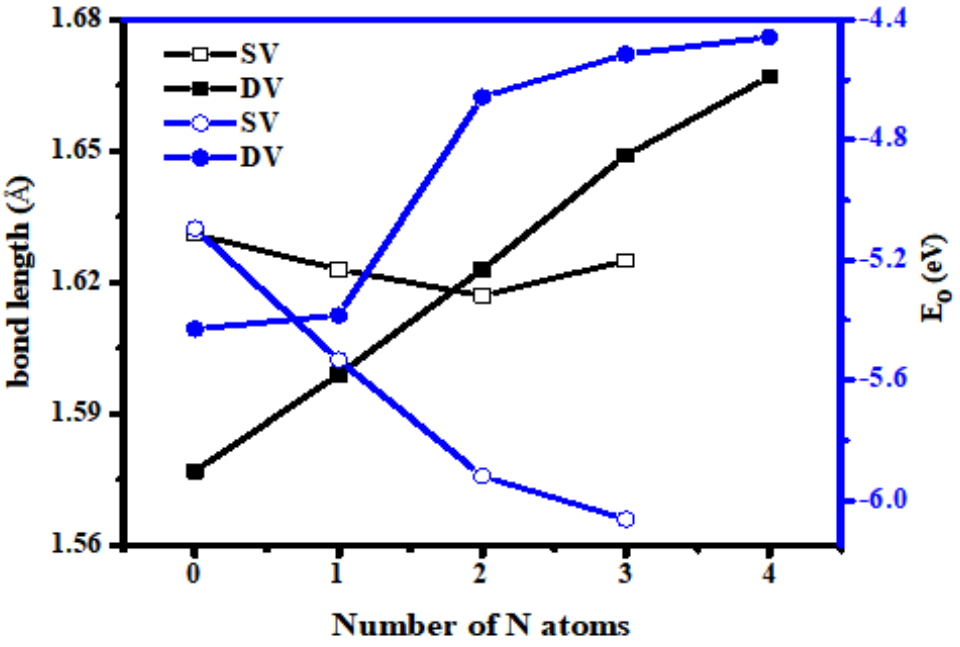

Figure S2. Bond length and E_O versus number of N atoms in single (SV) or double (DV) vacancy Fe-N doped structures

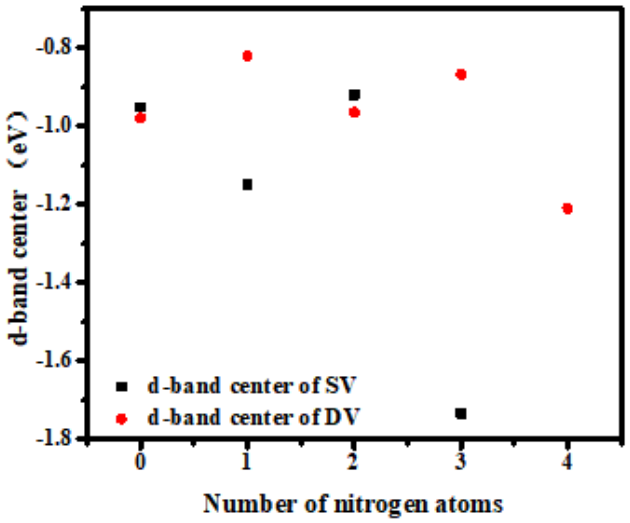

Figure S3. d-band center versus number of N atoms in single-double vacancy.