Supporting information

Size effect of oxygen reduction reaction on nitrogen-doped graphene quantum dots

Peng Zhang[1], Qiang Hu[1], Xuejing Yang[1], Xiuli Hou*[,1], Jianli Mi[1], Lei Liu[1],

Mingdong Dong*[,2]

1. Institute for Advanced Materials, School of Materials Science and Engineering, Jiangsu University, Zhenjiang 212013, China

2. Center for DNA Nanotechnology (CDNA), interdisciplinary Nanoscience Center (iNANO), Aarhus University, DK-8000 Aarhus, Denmark

**E-mail: houxiuli@ujs.edu.cn, dong@inano.au.dk*

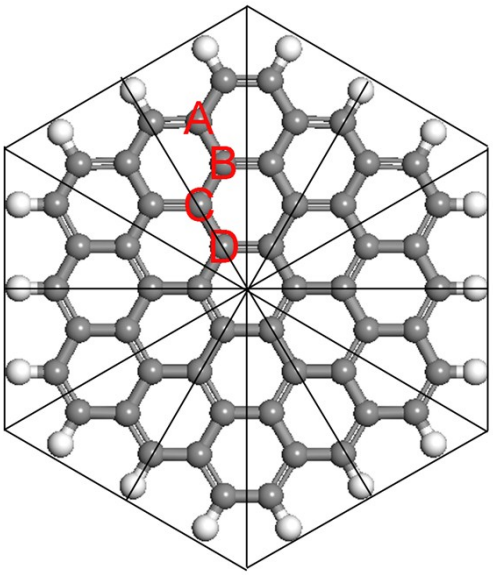

Figure S1. Schematic doped site of N atom in C53H18N.

Table S1. Relative energies of N-doped C53H18N with different doped sites.[a] All results are in unit of eV.

Site	A	B	C	D
Energy	0	0.15	0.26	0.23

[a] Here, we take m C53H18N as an example to study the favorable N doped site. As shown in Figure S1, the hexagonal GQD can be divided into 12 regions and the C atoms between different regions are equivalent. Thus, we only need to study the doped sites in one region. From Table S1, it is clear that Site A shows the lowest DFT energy, suggesting that Site A is the most favorable N-doped site.

Table S2. The calculated electronic energies (*E*), zero point energies (*ZPE*), and entropy values (*S*) of N-doped GQDs with adsorbed ORR intermediates. All results are in unit of eV.

	C23H12N	C23H12N +O_2	C23H12N +OOH	C23H12N +O	C23H12N +OH
E	-25535.441	-29632.584	-29649.851	-27584.781	-27601.947
ZPE	7.392	7.615	7.901	7.526	7.838
S	0.694	0.986	0.928	0.877	0.807
	C53H18N	C53H18N +O_2	C53H18N +OOH	C53H18N +O	C53H18N +OH
E	-56745.939	-60843.318	-60860.545	-58795.475	-58812.726
ZPE	14.232	14.458	14.768	14.340	14.697
S	1.580	1.578	1.622	1.543	1.528
	C95H24N	C95H24N +O_2	C95H24N +OOH	C95H24N +O	C95H24N +OH
E	-100402.294	-104499.688	-104516.903	-102451.838	-102469.109
ZPE	23.107	23.333	23.635	23.205	23.561
S	2.478	2.595	2.667	2.553	2.557
	C94H24N2	C94H24N2 +O_2	C94H24N2 +OOH	C94H24N2 +O	C94H24N2 +OH
E	-100855.052	-104952.742	-104969.685	-102904.963	-102921.880
ZPE	23.080	23.338	23.600	23.217	23.529
S	2.431	2.594	2.654	2.544	2.556
	C92H24N4	C92H24N4 +O_2	C92H24N4 +OOH	C92H24N4 +O	C92H24N4 +OH
E	-101760.567	-105858.310	-105875.086	-103810.594	-103827.268
ZPE	22.941	23.209	23.476	23.123	23.406
S	2.302	2.559	2.590	2.566	2.514

Table S3. The bond length of O-C bond ($d_{O\text{-}C}$) for adsorbed ORR intermediates on N-doped GQDs. All results are in unit of Å.

$d_{O\text{-}C}$	O_2	OOH	O	OH	H_2O
C23H12N	1.506	1.462	1.334	1.452	3.268
C53H18N	1.465	1.457	1.312	1.436	3.156
C95H24N	1.456	1.455	1.307	1.432	3.189
C94H24N2	1.434	1.456	1.307	1.434	3.221
C92H24N4	1.425	1.459	1.310	1.438	3.219