Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Optimizing Nitrogen Dopants in Carbon for Effective and Selective Two-Electron Water Oxidation to H_2O_2

Jiaxiang Qiu,[a] Jinlong Wu,[a] Zhongti Sun,[a] Ying Wang,*[b] and Yangyang Wan*[a]

[a] School of Materials Science and Engineering, Jiangsu University, Zhenjiang 212013, China

[b] School of Physics and Electronic Engineering, Jiangsu University, 212013, Zhenjiang, China.

*Email: yingwang24@ujs.edu.cn, yangyang.wan@ujs.edu.cn

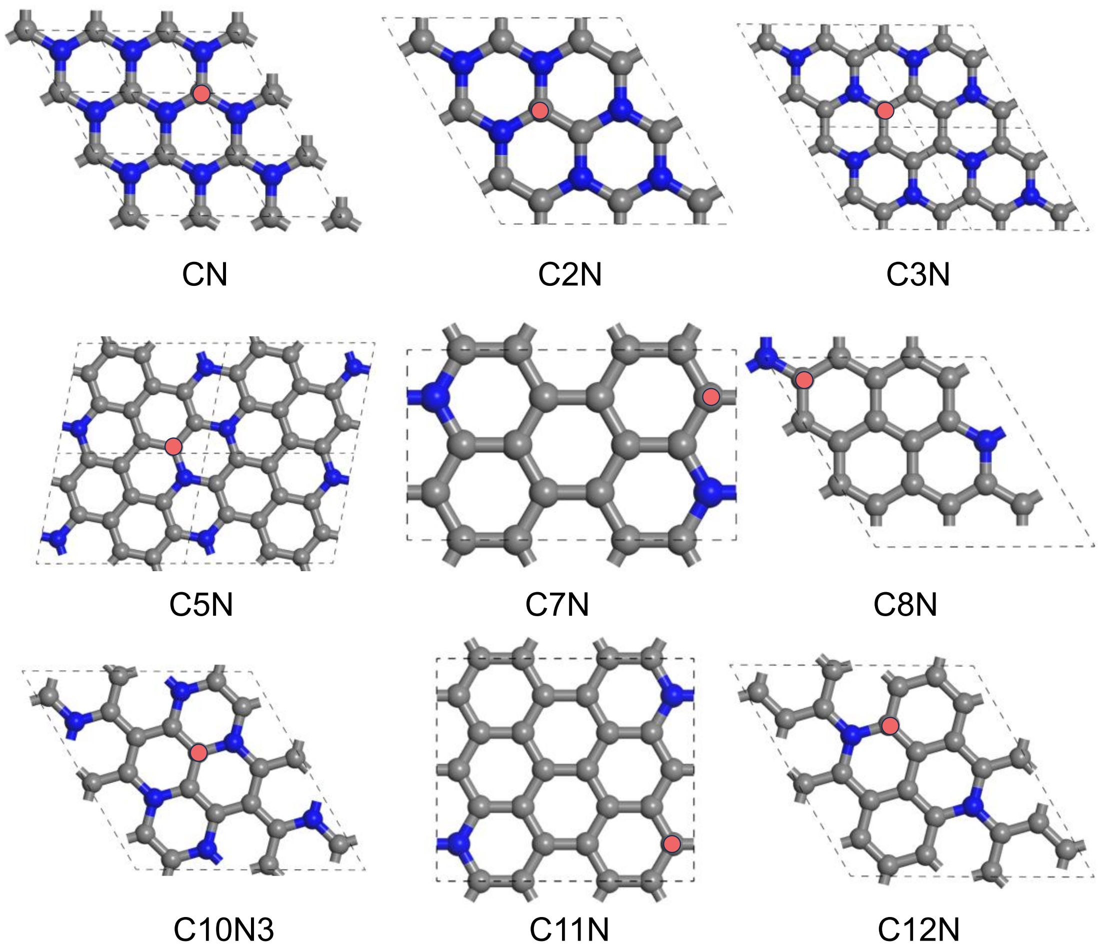

Figure S1. Optimized structures of graphitic 2D CNs, where the red dots represent the most stable adsorbed sites for OH and O.

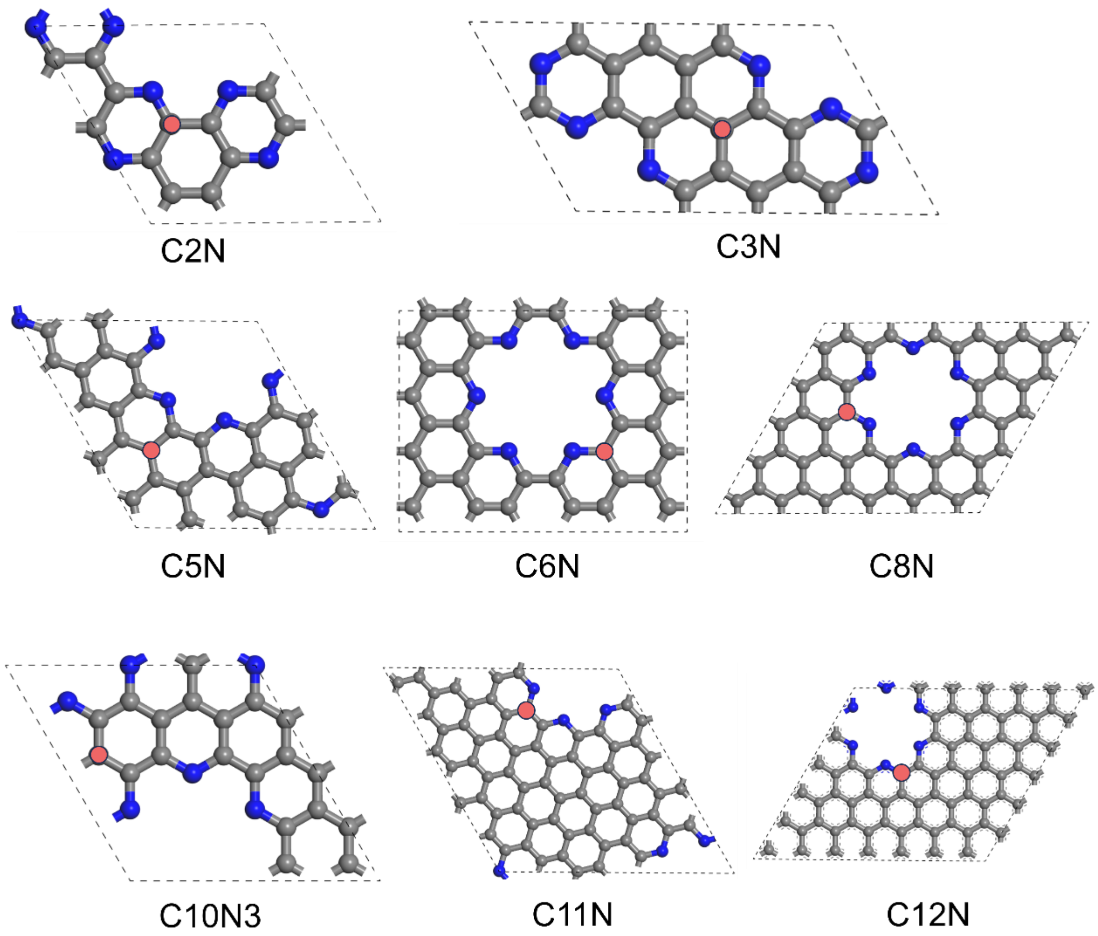

Figure S2. Optimized structures of pyridinic 2D CNs, where the red dots represent the most stable adsorbed sites for OH and O.

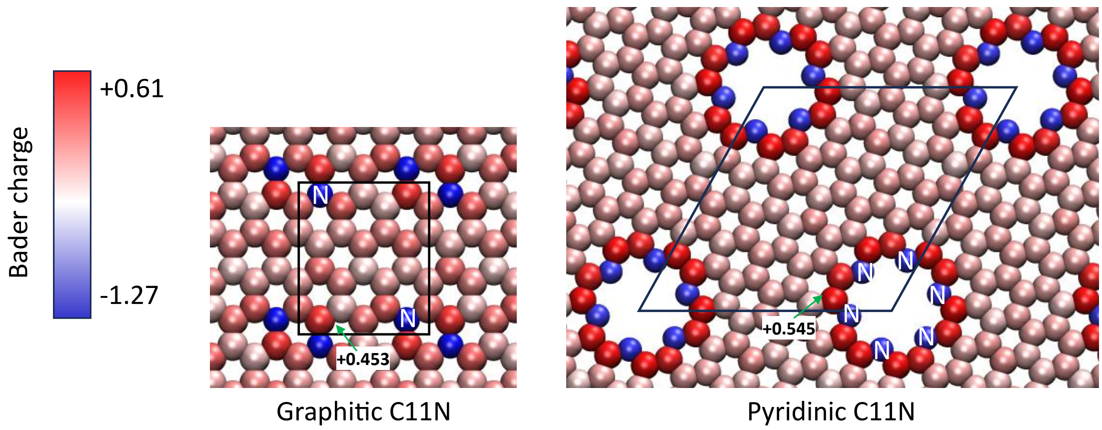

Figure S3. Bader charge analysis of C11N.

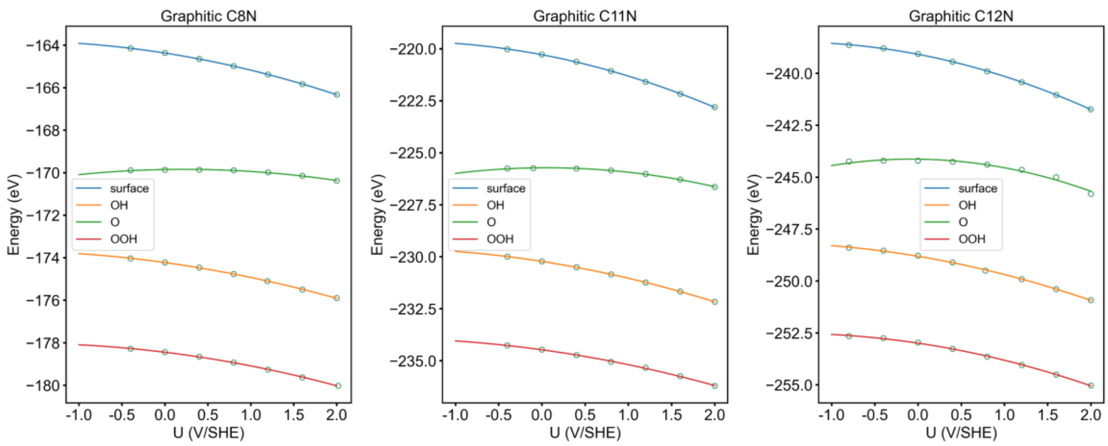

Figure S4. The fitting energies of bare surface and absorbed intermediate states as a function of applied potential for graphitic C8N, C11N and C12N, respectively.

Table S1. The lattice constant, atoms in unit cell and supercell used for intermediates adsorption computation of graphitic CN and pyridinic models.

Graphitic CN	Lattice constant	Atoms	Supercell
CN	a=b=2.396Å; α=90°, β=90°, γ=120°	2	4×4×1
C2N	a=b=7.253Å; α=90°, β=90°, γ=120°	18	1×1×1
C3N	a=b=4.861Å; α=90°, β=90°, γ=120°	8	2×2×1
C5N	a=4.887Å b=6.458Å; α=90°, β=90°, γ=101°	12	2×2×1
C7N	a=4.900Å b=8.472Å; α=90°, β=90°, γ=90°	16	2×1×1
C8N	a=b=7.349Å; α=90°, β=90°, γ=120°	18	1×1×1
C10N3	a=b=8.767Å; α=90°, β=90°, γ=120°	26	1×1×1
C11N	a=7.361Å b=8.504Å; α=90°, β=90°, γ=120°	24	1×1×1
C12N	a=b=8.852Å; α=90°, β=90°, γ=120°	26	1×1×1

Pyridinic CN	Lattice constant	Atoms per unit cell	Supercell
graphene	a=b=2.467Å; a=90°, b=90°, g=120°	2	4×4×1
C2N	a=b=8.322Å; α=90°, β=90°, γ=120°	18	1×1×1
C3N	a=7.295Å b=12.077Å; α=90°, β=90°, γ=120°	24	1×1×1
C5N	a=b=11.167Å; α=90°, β=90°, γ=120°	36	1×1×1
C6N	a=9.767Å b=12.685Å; α=90°, β=90°, γ=90°	42	1×1×1
C8N	a=12.249Å b=14.686Å; α=90°, β=90°, γ=120°	54	1×1×1
C10N3	a=b=9.702Å; α=90°, β=90°, γ=120°	26	1×1×1
C11N	a=b=15.314Å; α=90°, β=90°, γ=120°	72	1×1×1
C12N	a=14.723Å b=17.176Å; α=90°, β=90°, γ=120°	78	1×1×1