Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Pyrrolic-nitrogen doped graphene: a metal-free electrocatalyst with high efficiency and selectivity for the reduction of carbon dioxide to formic acid: a computational study

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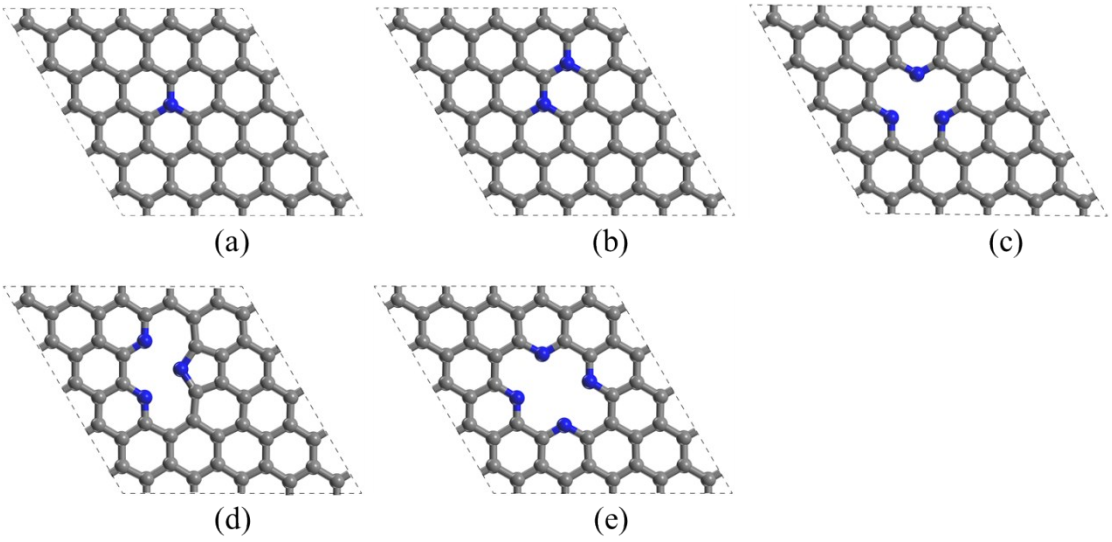

Figure S1. The optimized structures of different N-doped graphenes: (a) graphN1, (b) graphN2, (c) pyriN3, (d) pyrroN3, and (e) pyriN4. The gray and blue balls represent the C and N atoms, respectively.

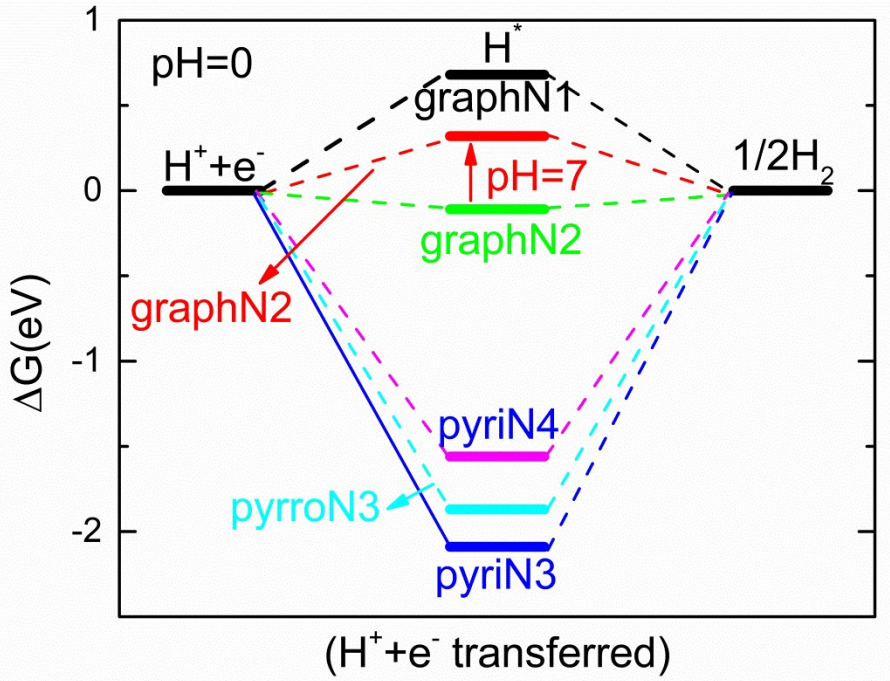

Figure S2. Free energy diagram of HER on various N−doped graphenes.

Table S1. The N content, shortest C-N bond length ($d_{C\text{-}N}$, Å) and formation energies (E_f, eV) of different N-doped graphenes.

	graphN1	graphN2	pyriN3	pyrroN3	pyriN4
N, wt %	2.33	4.64	7.07	7.07	9.59
$d_{C\text{-}N}$	1.408	1.398	1.338	1.323	1.330
E_f	0.83	2.05	3.30	5.71	3.67