Electronic Supplementary Material (ESI) for RSC Advances.

Table S1: Comparison of the binding energies (E_b) for Pt_{13} cluster on N-doped graphene with 3NV structure on (a) different supercell or (b) with different k-points.

(a)

supercell size	E_b
5 × 5	-6.495
6 × 6	-6.492
7 × 7	-6.491

(b)

k-point density	E_b
2 × 2 × 1	-6.495
3 × 3 × 1	-6.495
4 × 4 × 1	-6.496
5 × 5 × 1	-6.496
6 × 6 × 1	-6.496
7 × 7 × 1	-6.496

Table S2: Adsorption energies and structural parameters of O on deposited Pt_{13} clusters on N-doped graphene with (a) N_C, (b) 3NV, and (c) 4ND structures.

site	E_{ads}	d_{Pt-O}
Pt1	-0.914	1.822
Pt1-Pt2	-1.458	1.939
Pt1-Pt12	-1.473	1.918
Pt1-Pt5	-1.028	1.954
Pt1-Pt5-Pt8	-1.196	2.034
Pt1-Pt8	-1.121	1.952
Pt1-Pt12	-1.494	1.919
Pt2	-1.320	1.785
Pt2-Pt3	-1.123	1.988
Pt2-Pt6-Pt13	-0.890	2.019
Pt2-Pt7	-1.196	1.917
Pt2-Pt6	-1.143	1.953
Pt3	-1.383	1.919
Pt3-Pt4-Pt10	-1.052	2.022
Pt3-Pt4-Pt12	-1.088	1.969
Pt3-Pt6	-1.721	1.987
Pt3-Pt10	-1.285	1.934
Pt3-Pt12	-1.410	1.921
Pt4-Pt5	-1.101	1.917
Pt4-Pt5-Pt9	-1.130	1.988
Pt4-Pt9-Pt10	-1.141	2.088
Pt4-Pt10	-1.410	1.973
Pt4-Pt12	-1.060	1.908
Pt5	-1.310	1.797
Pt5-Pt8	-1.385	1.592
Pt5-Pt9	-1.174	1.898
Pt6	-1.180	1.800
Pt6-Pt13	-1.762	1.964
Pt7	-1.114	1.783
Pt7-Pt8	-1.512	1.920
Pt7-Pt13	-1.254	1.907
Pt8	-0.656	1.822
Pt11-Pt13	-0.523	1.922
Pt12	-1.370	1.782

(b)

site	E_{ads}	$d_{Pt\text{-}O}$
Pt1	-0.492	1.801
Pt1-Pt2	-1.508	1.956
Pt1-Pt5-Pt8	-1.310	2.052
Pt1-Pt7	-0.772	1.988
Pt1-Pt8	-1.452	1.967
Pt1-Pt12	-0.531	1.911
Pt2	-0.634	1.801
Pt2-Pt3	-1.110	1.967
Pt2-Pt12	-0.298	1.945
Pt3-Pt4	-0.466	1.909
Pt3-Pt6	-0.844	1.954
Pt3-Pt12	-1.070	1.940
Pt4	-0.545	1.788
Pt4-Pt5	-0.871	1.965
Pt4-Pt10	-0.792	1.955
Pt4-Pt12	-1.170	1.959
Pt5	-0.564	1.788
Pt5-Pt8	-1.138	1.915
Pt5-Pt9	-0.742	1.953
Pt5-Pt9-Pt10	-0.330	1.966
Pt5-Pt12	-1.186	1.932
Pt6	-0.922	1.797
Pt6-Pt10	-1.653	1.973
Pt8	-0.439	1.811
Pt8-Pt9	-1.210	1.968
Pt8-Pt13	-1.723	1.957
Pt9	-0.596	1.788
Pt9-Pt10	-1.365	1.954
Pt9-Pt13	-0.817	1.924
Pt10	-0.477	1.805
Pt10-Pt13	-0.808	2.017
Pt12	-0.800	1.788

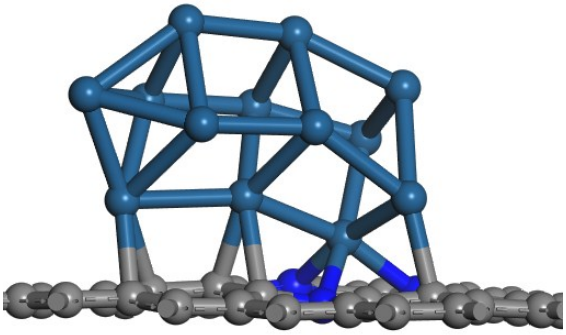
(c)

site	E_{ads}	d_{Pt-O}
Pt1-Pt2	-0.371	1.967
Pt1-Pt2-Pt6	-0.695	1.988
Pt1-Pt2-Pt12	-0.486	2.071
Pt1-Pt5	-1.256	1.965
Pt1-Pt5-Pt8	-0.172	2.011
Pt1-Pt5-Pt12	-0.481	2.017
Pt1-Pt6	-0.543	1.930
Pt1-Pt7	-0.794	1.933
Pt1-Pt7-Pt8	-0.662	2.014
Pt1-Pt2-Pt12	-0.618	2.056
Pt2	-0.997	1.786
Pt2-Pt3	-1.038	1.954
Pt2-Pt3-Pt6	-0.691	1.974
Pt2-Pt3-Pt12	-0.732	2.056
Pt2-Pt6	-1.284	1.974
Pt2-Pt12	-1.394	1.957
Pt3-Pt4	-1.079	1.940
Pt3-Pt4-Pt10	-0.532	2.005
Pt3-Pt4-Pt12	-0.415	2.002
Pt3-Pt6	-0.741	1.937
Pt3-Pt12	-0.769	1.953
Pt4	-0.649	1.794
Pt4-Pt9	-1.169	1.954
Pt4-Pt9-Pt12	-0.913	2.082
Pt4-Pt10	-0.825	1.936
Pt4-Pt12	-0.702	1.972
Pt5	-1.195	1.783
Pt5-Pt8	-1.200	1.975
Pt5-Pt8-Pt9	-0.660	1.992
Pt5-Pt9	-1.507	1.973
Pt5-Pt12	-0.928	1.957
Pt6	-1.286	1.976
Pt6-Pt7	-1.115	1.951
Pt7	-0.156	1.799
Pt8	-0.800	1.809
Pt9	-1.091	1.780
Pt9-Pt12	-0.706	1.945
Pt12	-0.517	1.796

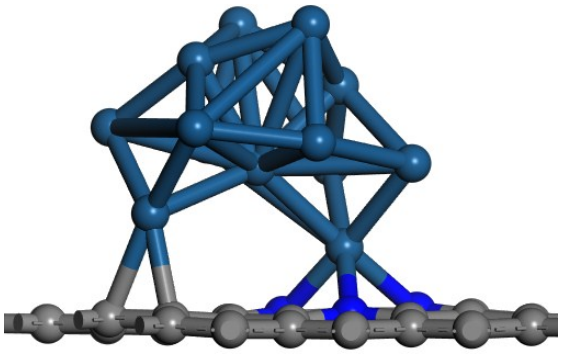
Figure S1. The most stable configurations and binding energies of Pt_{13} clusters with C_{4v}, D_{5h}, O_h, and I_h symmetry structures and the low energy structure on N-doped graphene with the 3NV structure.

Figure S2. The PDOS of (a) free Pt_{13} and the Pt atoms far away from interface in the supported Pt_{13} clusters on (b) N_C, (c) 3NV, and (d) 4ND. The Fermi level is set as zero

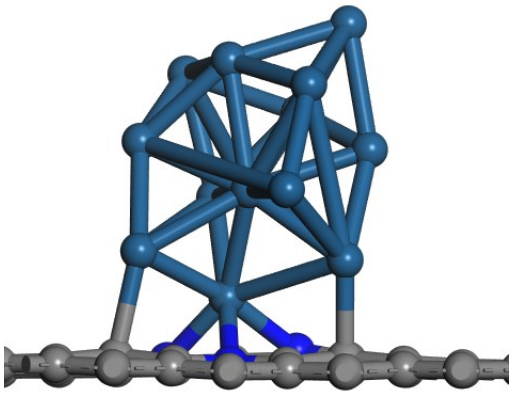
Figure S1



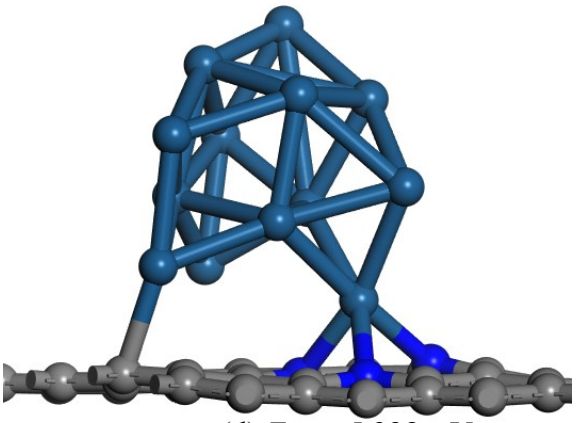
(a) E_b = −4.200 eV



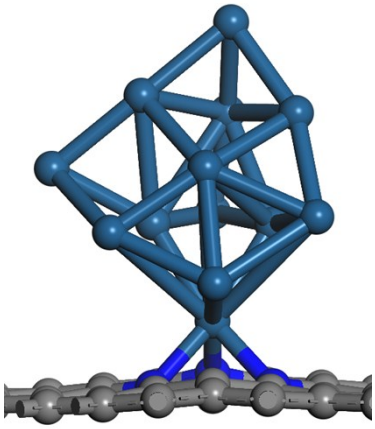
(b) E_b = −5.856 eV



(c) E_b = −4.919 eV

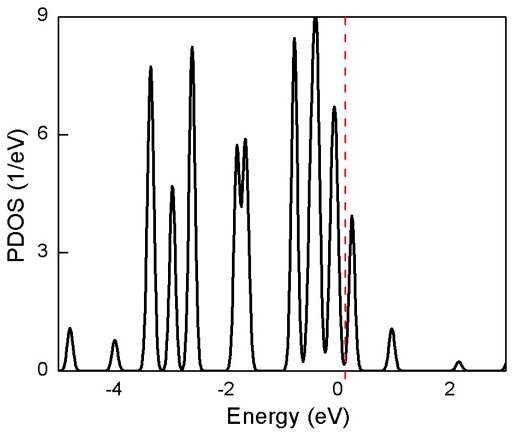


(d) E_b = −5.328 eV

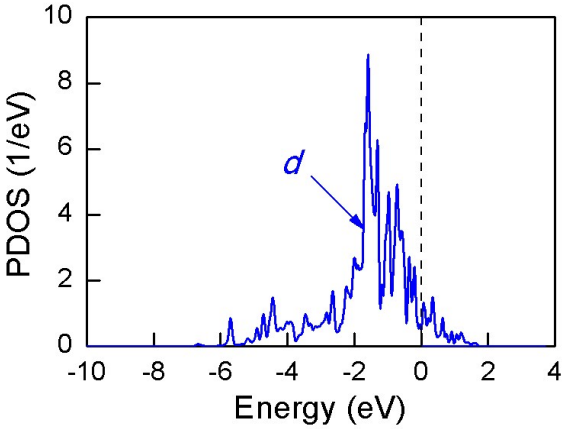


(e) E_b = −6.848 eV

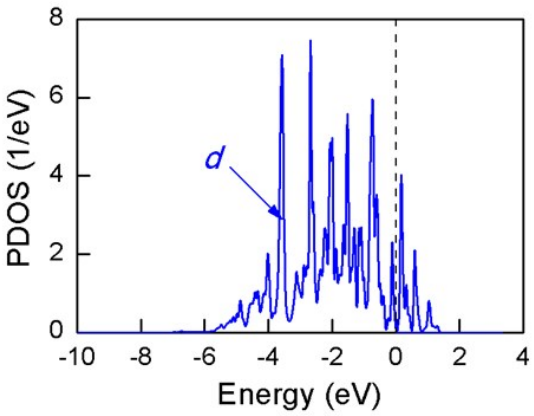
Figure S2



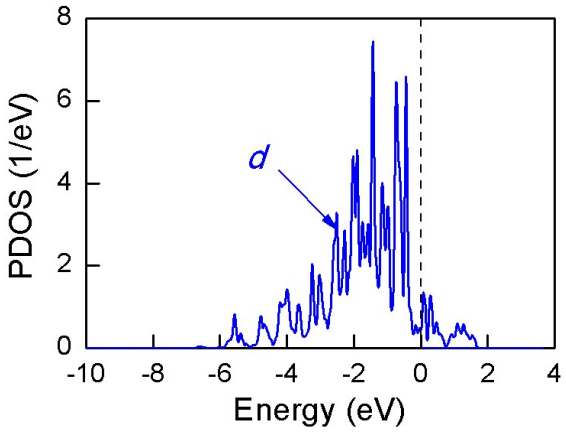
(a)



(b)



(c)



(d)