**Supporting Information**

# $Pt_3$ Cluster Anchored on $C_2N$ Monolayer as an Efficient Catalyst for Electrochemical Reduction of Nitrobenzene to Aniline: a Computational Study

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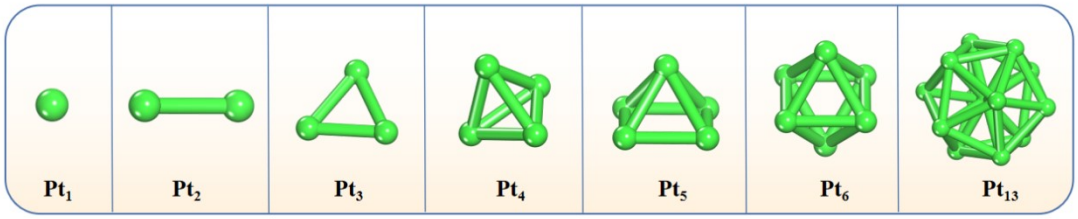


**Fig. S1** The optimized models of the $Pt_n$ (n = 1~6, 13) clusters.

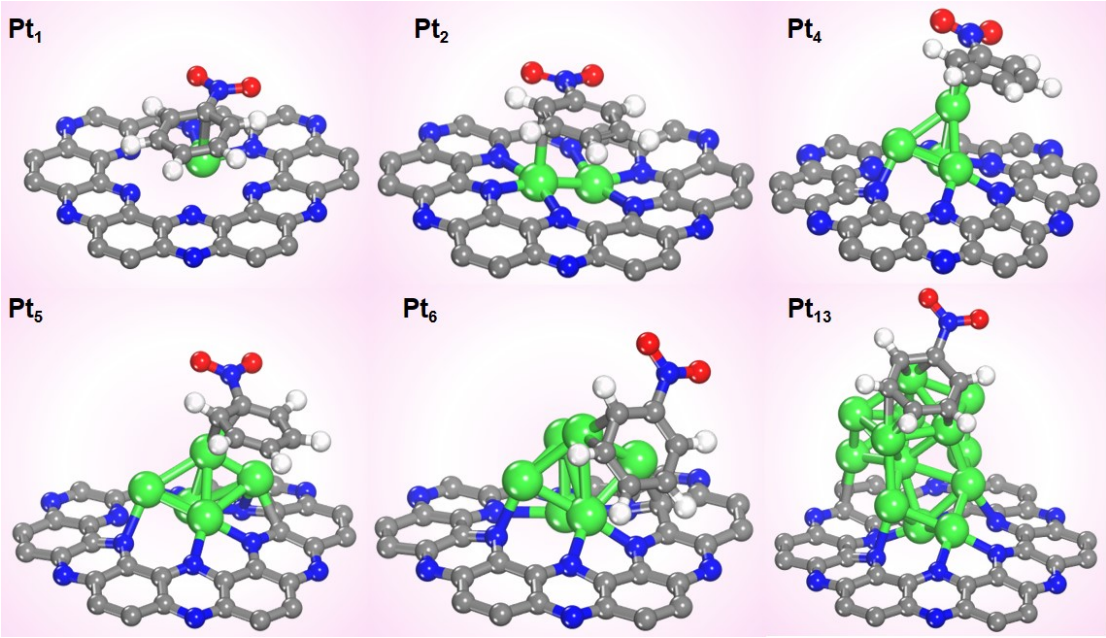


**Fig. S2** The most stable adsorption configurations of Ph-$NO_2$ on the surface of $Pt_n/C_2N$ ($Pt_n$, n = 1, 2, 4~6 and 13). The green, blue, red and gray balls represent Pt, N, O and C atoms, respectively.

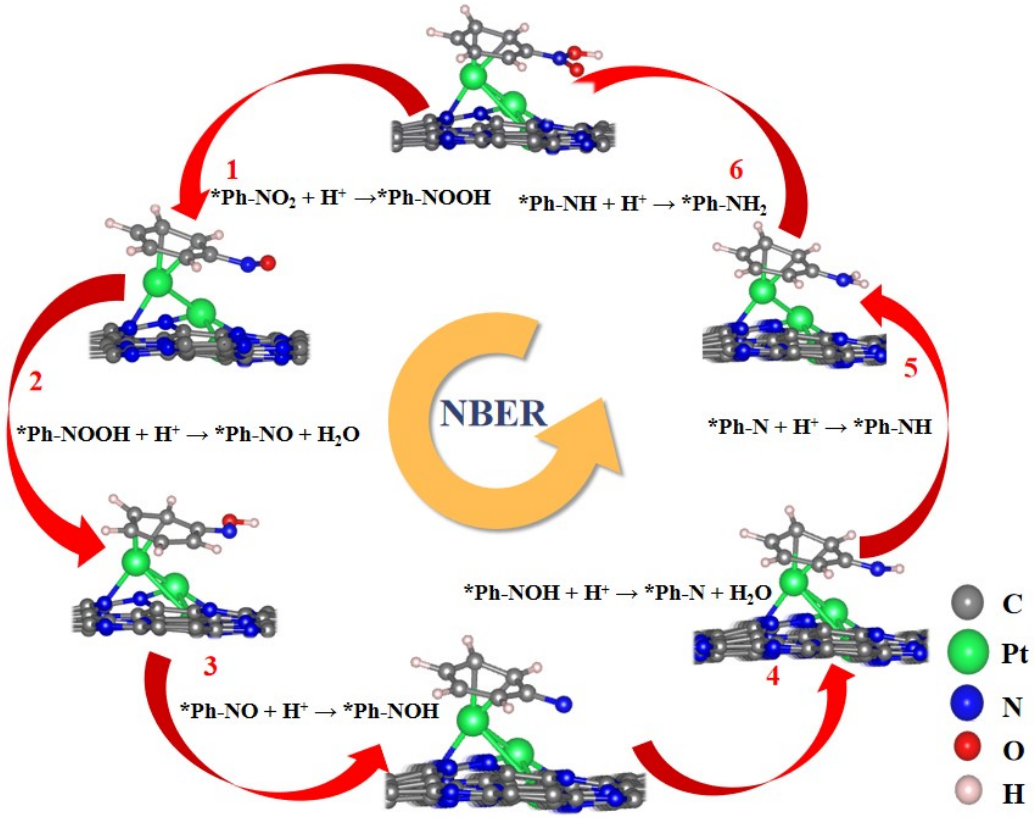


**Fig. S3** The optimal path and intermediates involved in the electroreduction of Ph-$NO_2$ to Ph-$NH_2$ on the surface of $Pt_3/C_2N$: Ph-NOOH$^*$, Ph-NO$^*$, Ph-NOH$^*$, Ph-N$^*$, Ph-NH$^*$, and Ph-$NH_2$$^*$.