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

Improving the Photocatalytic Activity of s-triazine Based Graphitic Carbon Nitride through Metal Decoration: An *ab initio* Investigation

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Table S1: The calculated energy difference between the impurity state maximum and Fermi level (Δ(I-F)) and Fermi level and Conduction band minimum (Δ(F-C)) from the HSE03 functional.

System	Δ(I-F)	Δ(F-C)
PCN-Sc	0.14	0.16
PCN-Ti	0.15	0.02
PCN-V	0.22	0.22
PCN-Cr	0.09	0.09
PCN-Mn	0.09	0.12
PCN-Fe	0.11	0.15
PCN-Co	0.27	0.33
PCN-Ni	0.15	0.15
PCN-Cu	0.11	0.12
PCN-Zn	0.24	0.24
PCN-Ag	0.06	0.06
PCN-Au	0.06	0.07
PCN-Pt	0.24	0.37
PCN-Pd	0.10	0.11

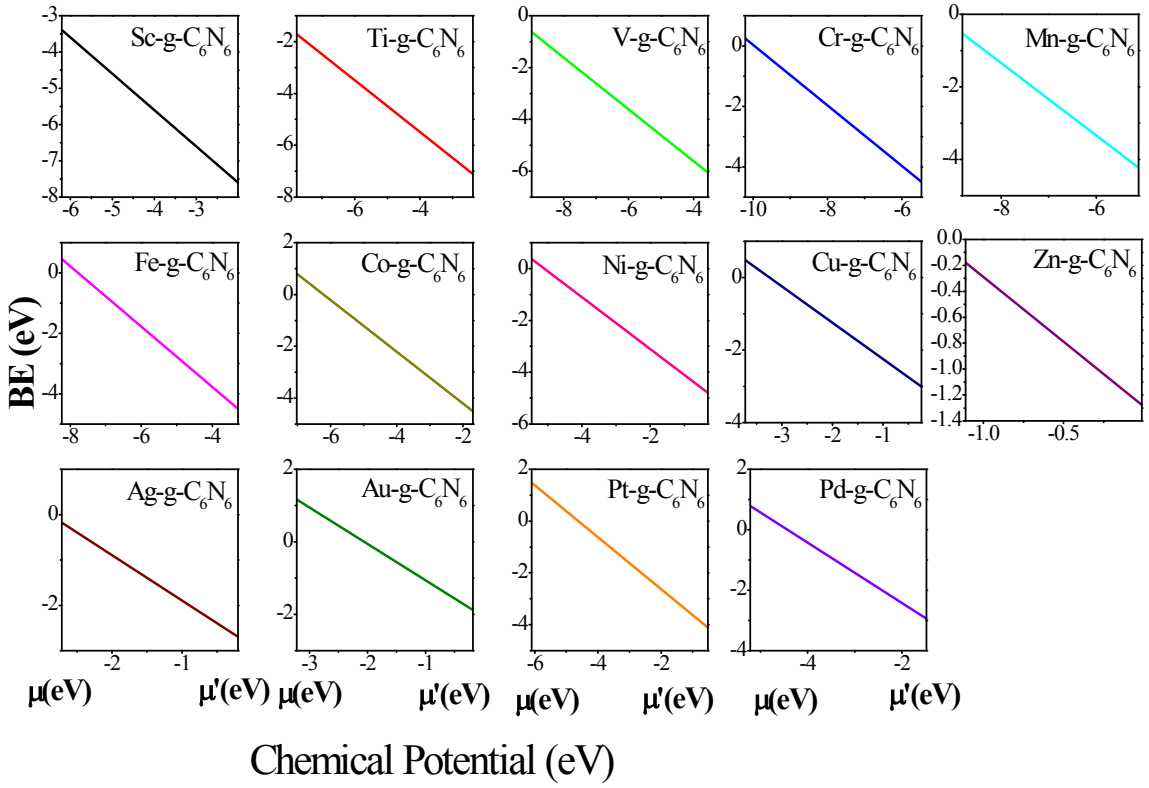

Figure S1: Variation of metal binding energy to the g-C_3N_3 surface with the chemical potential of the metal varied from bulk metal to isolated metal atom.