Supporting Information

"Gating Effect" of g-C3N4 Encapsulated Pt-based Catalysts for Hydrogenation and Bamberger Rearrangement of Nitroaromatics

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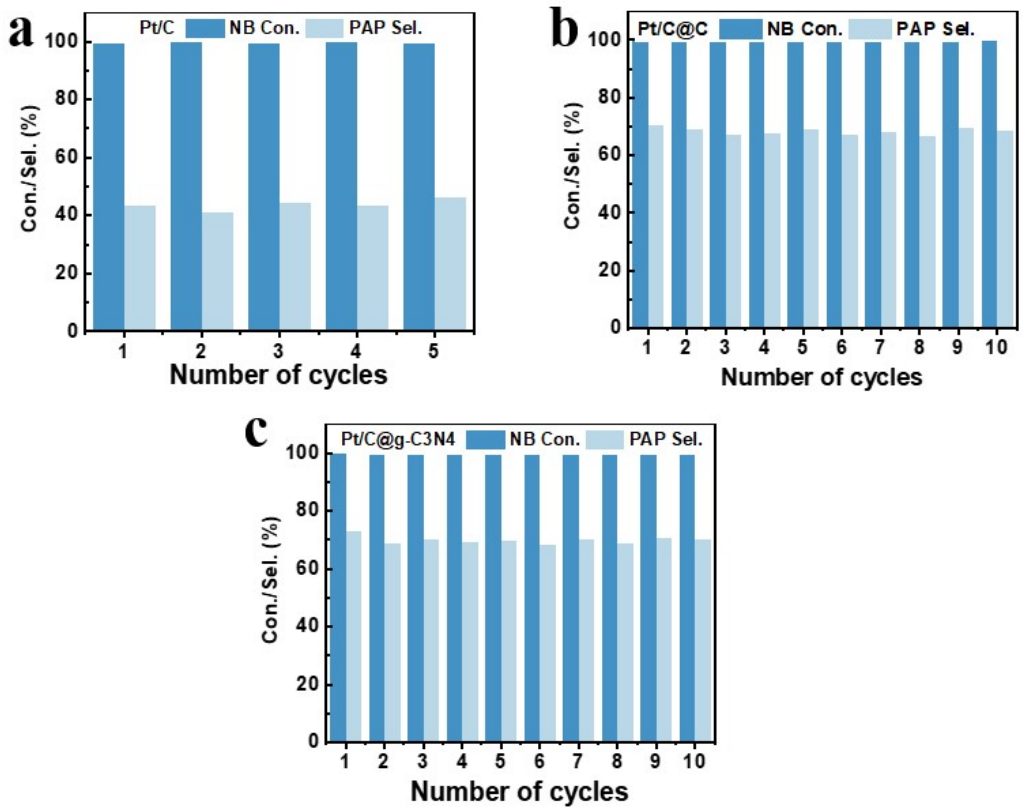

Fig. S1 Catalyst performance and stability testing of a) Pt/C, b) Pt/C@C and c) Pt/C@g-C_3N_4.

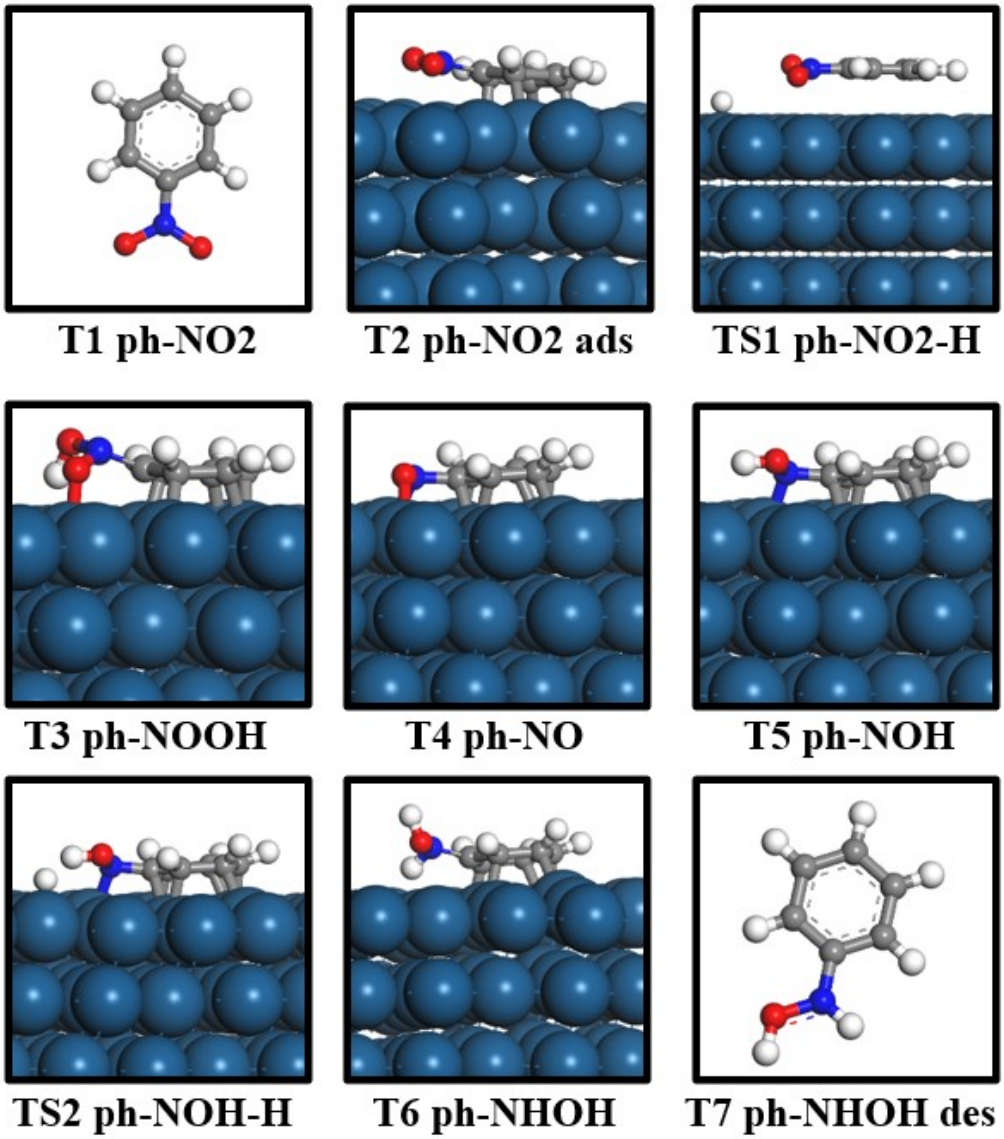

Fig. S2 The elemental reaction steps of intermediates on the Pt/C surface. T1: ph-NO_2, T2: ph-NO_2 adsorption, TS1: ph-NO_2-H, T3: ph-NOOH, T4: ph-NO, T5: ph-NOH, TS2: ph-NOH-H, T6: ph-NHOH, T7: ph-NHOH desorption.

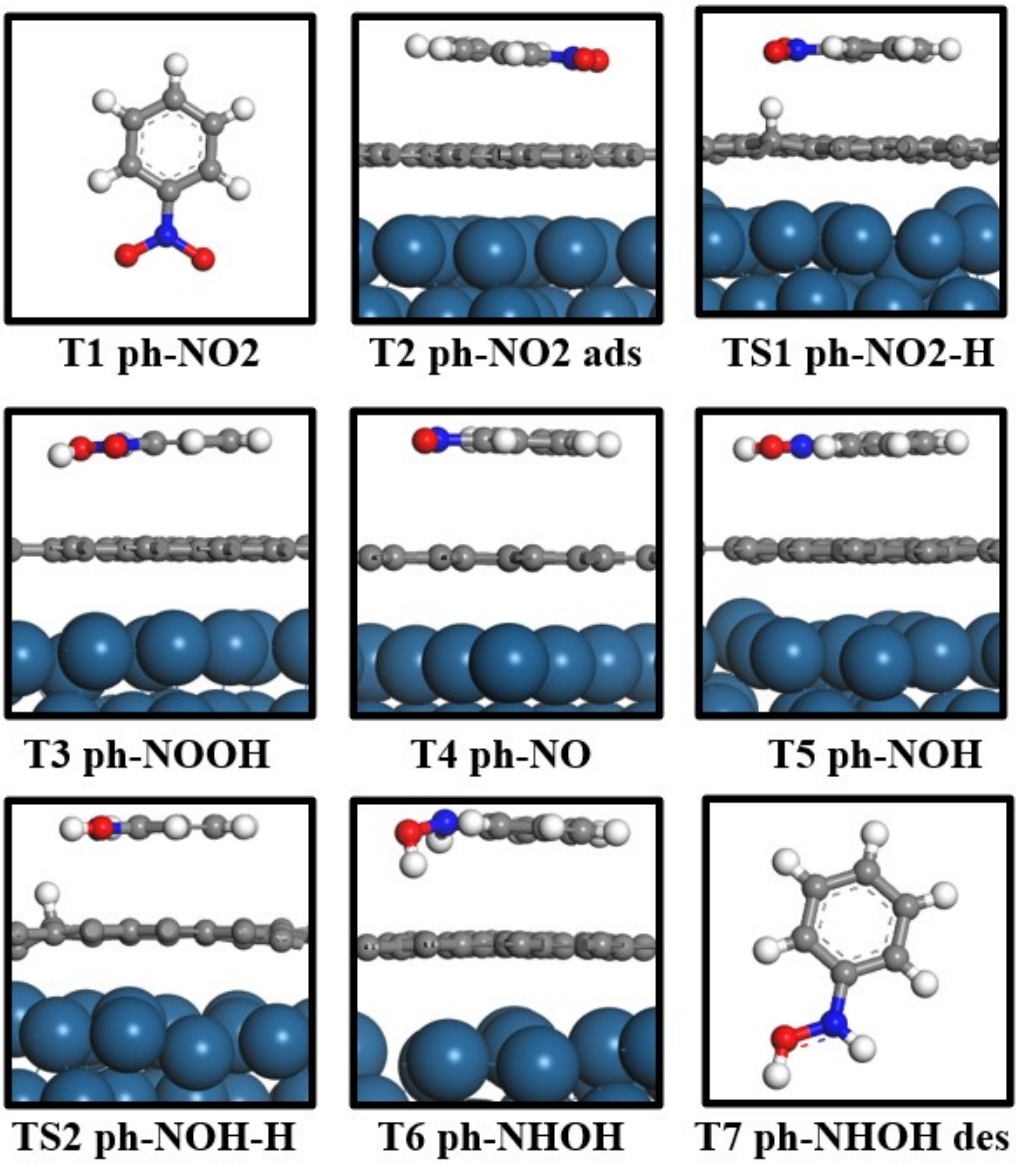

Fig. S3 The elemental reaction steps of intermediates on the Pt/C@C surface. T1: ph-NO_2, T2: ph-NO_2 adsorption, TS1: ph-NO_2-H, T3: ph-NOOH, T4: ph-NO, T5: ph-NOH, TS2: ph-NOH-H, T6: ph-NHOH, T7: ph-NHOH desorption.

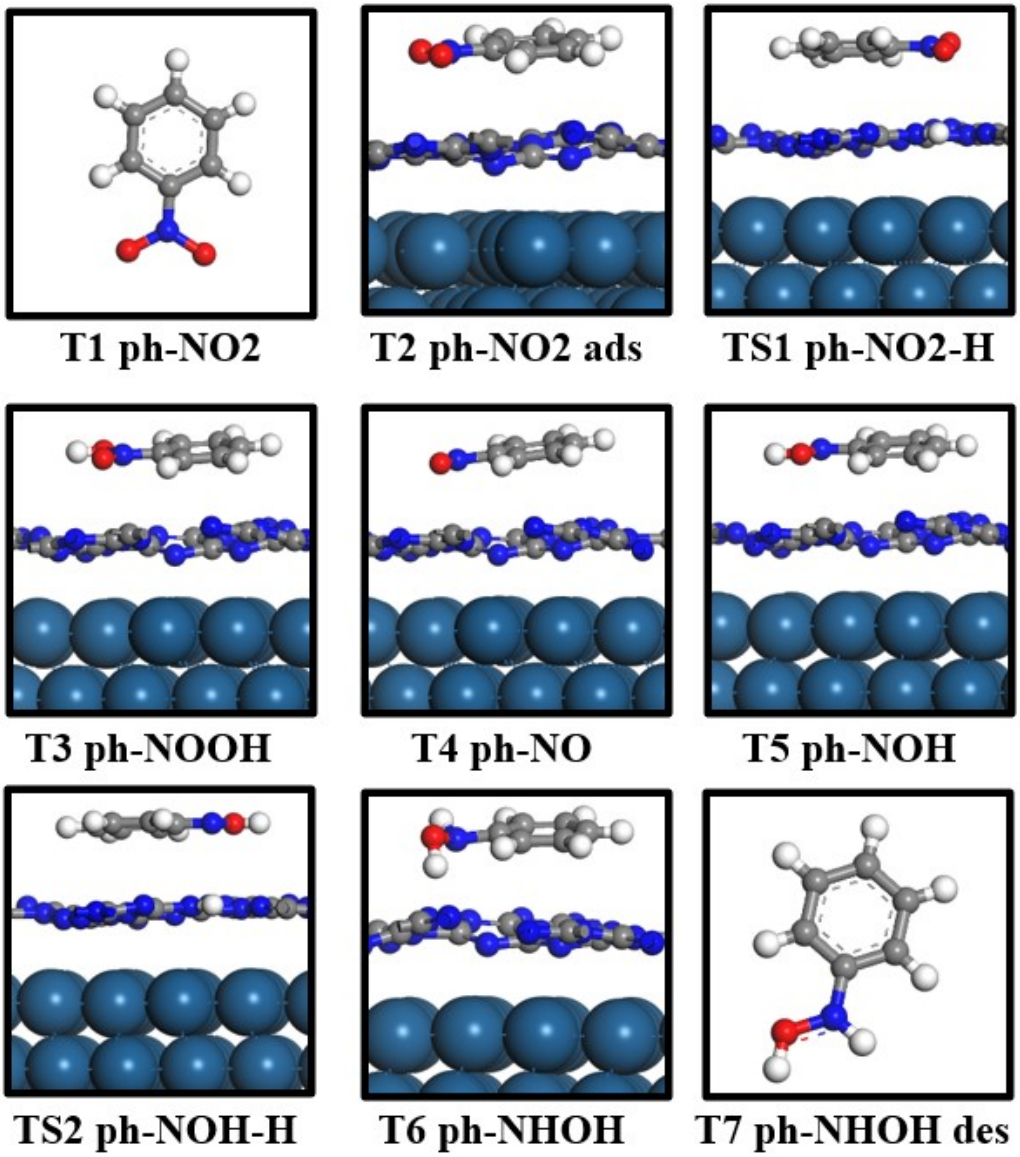

Fig. S4 The elemental reaction steps of intermediates on the Pt/C@g-C_3N_4 surface. T1: ph-NO_2, T2: ph-NO_2 adsorption, TS1: ph-NO_2-H, T3: ph-NOOH, T4: ph-NO, T5: ph-NOH, TS2: ph-NOH-H, T6: ph-NHOH, T7: ph-NHOH desorption.

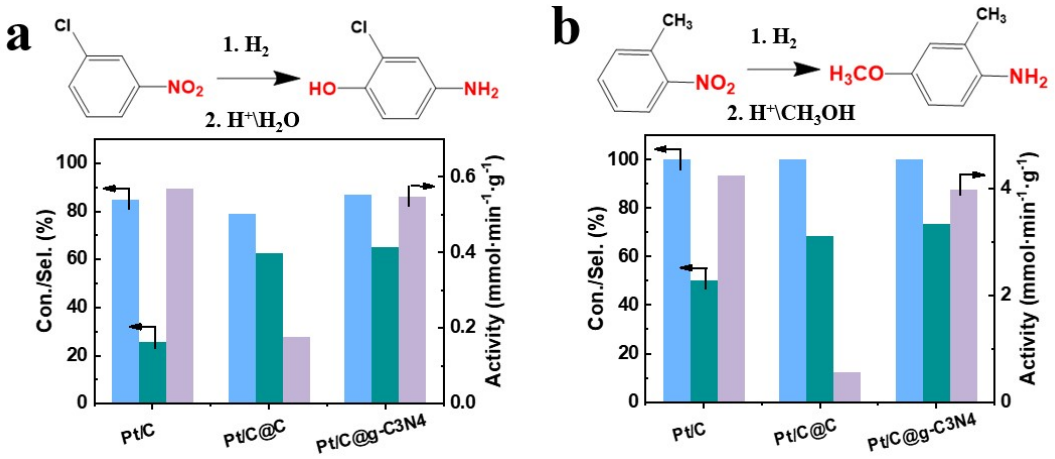

Fig. S5 Nitroaromatics hydrogenation-Bamberger rearrangements of a) 1-chloro-3-nitrobenzene and H_2O, b) 2-nitrotoluene and CH_3OH.

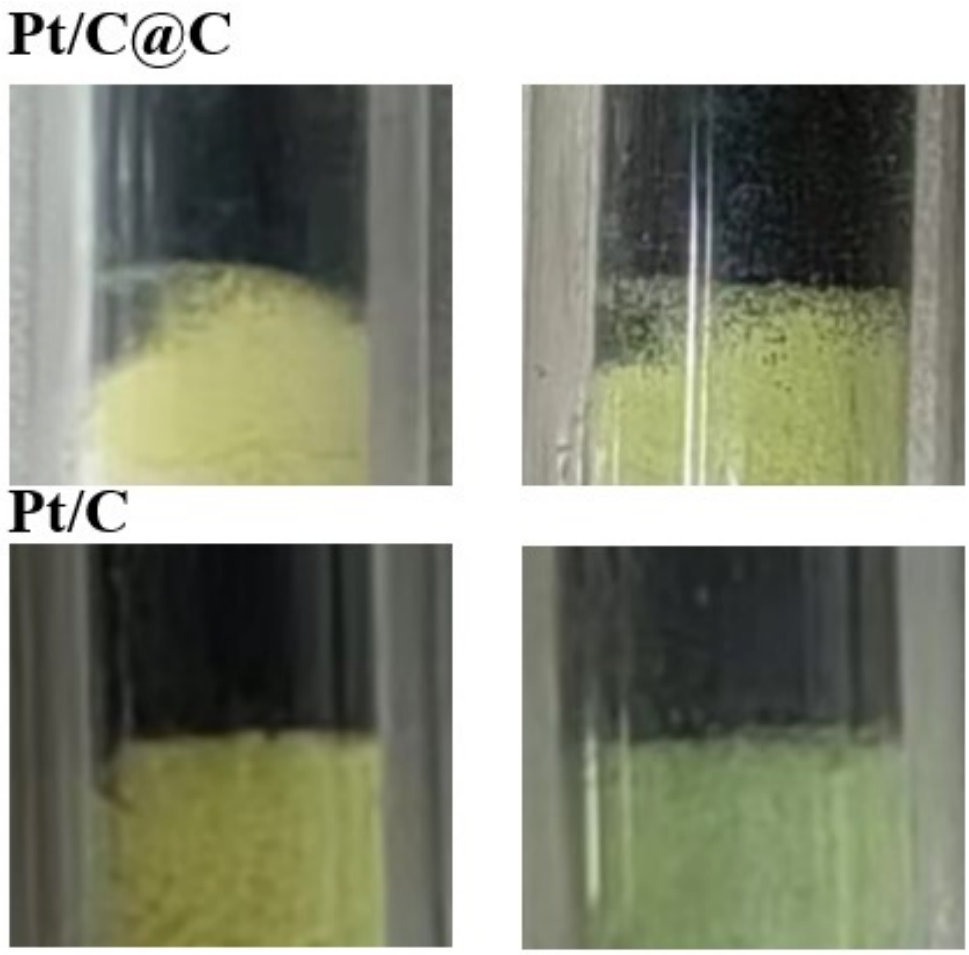

Fig. S6 Experiment on color change of WO_3 upon hydrogen spillover reduction.

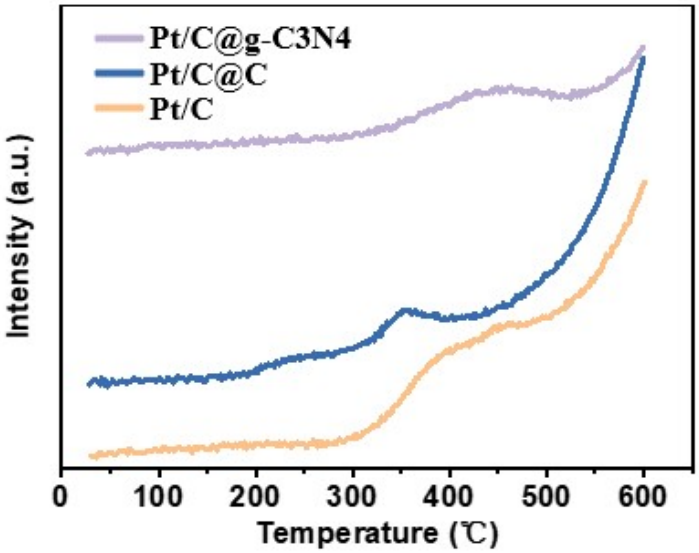

Fig. S7 H_2-TPD-MS results of Pt/C, Pt/C@C, and Pt/C@g-C_3N_4.

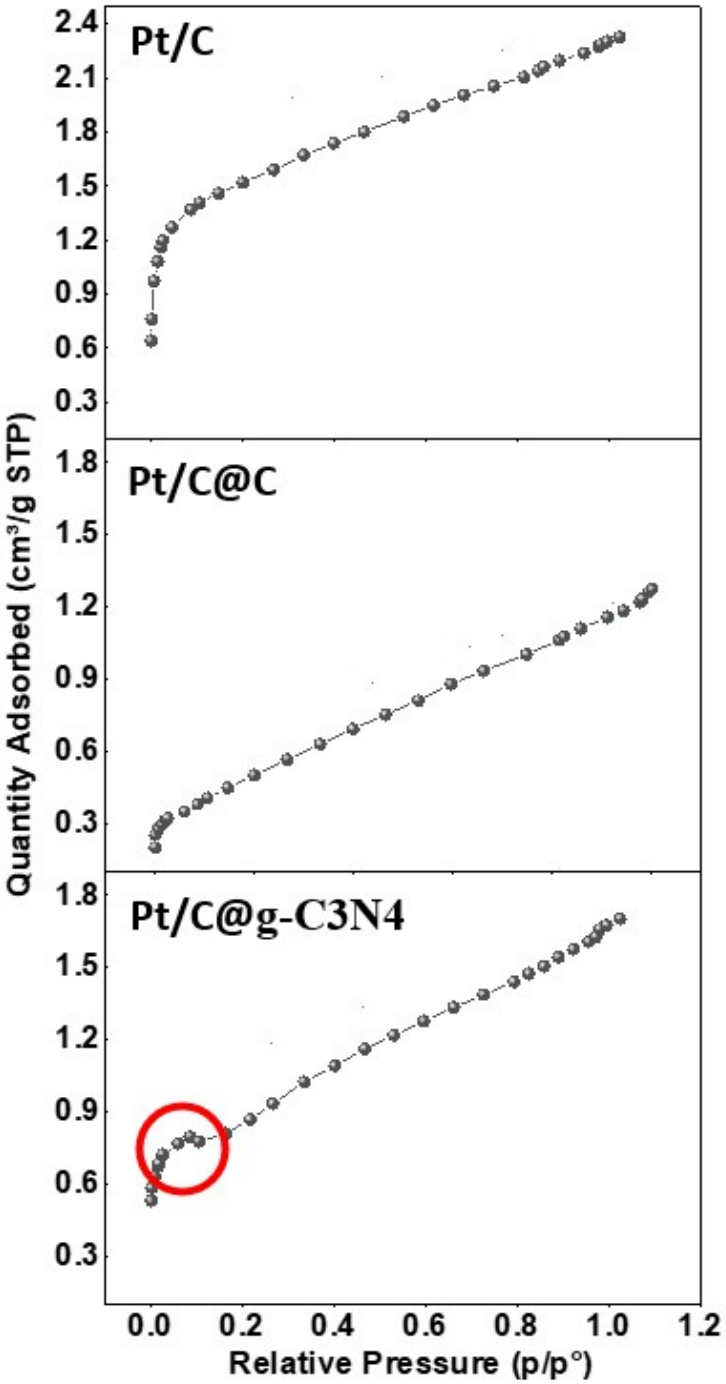

Fig. S8 BET results of H_2 adsorption curves for Pt/C, Pt/C@C, and Pt/C@g-C_3N_4.

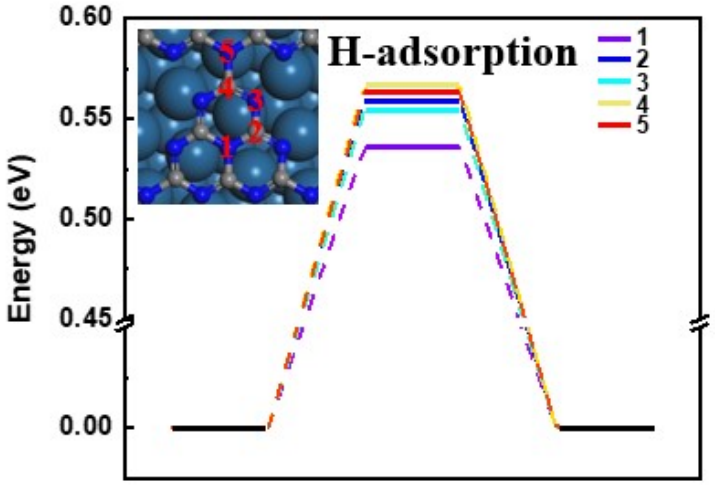

Fig. S9 The H_2 dissociation energy of different adsorption sites on the Pt/C@g-C_3N_4 surface g-C_3N_4.

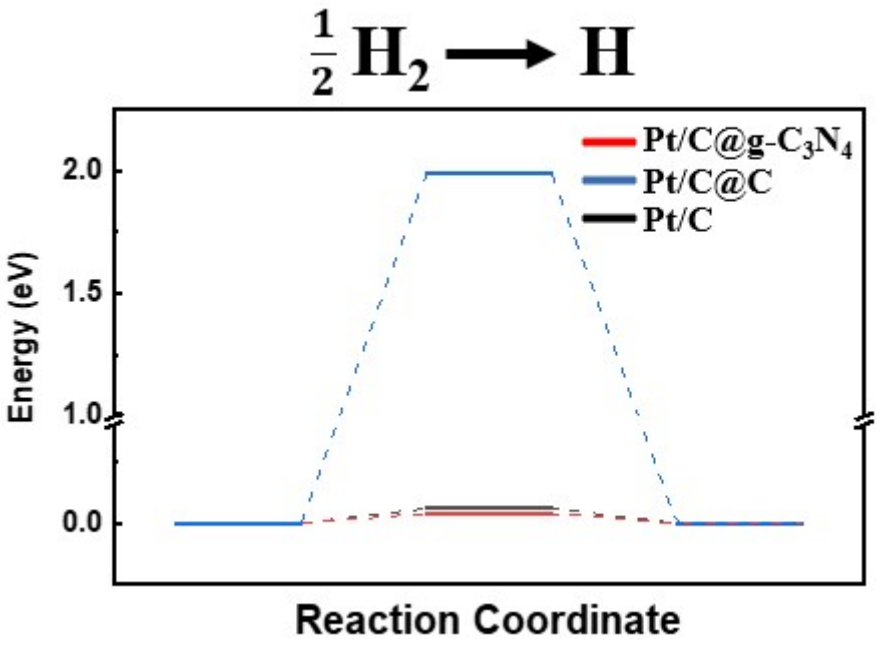

Fig. S10 The H_2 dissociation energy of Pt/C, Pt/C@C, and Pt/C@g-C_3N_4.

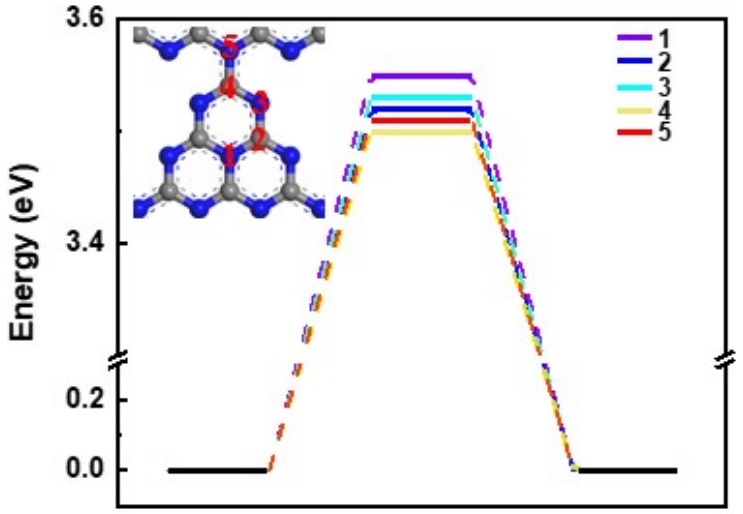

Fig. S11 The H_2 dissociation energy of different adsorption sites on the pure g-C_3N_4 surfaces.