

Exploring Deactivation Reasons of Biomass-Based Phosphorus-Doped Carbon as a Metal-Free Catalyst in the Catalytic Dehydroaromatization of *n*-heptane
Supplementary Information

Fei Yu ^{1,2}, Siyuan Liu ^{1*} and Bo Liu ¹

¹ *Green Chemical Engineering Research Center, Shanghai Advanced Research Institute, Chinese Academy of Sciences, Shanghai 201210, China.*

² *University of Chinese Academy of Sciences, Beijing 100049, China*

liusiyuan@sari.ac.cn

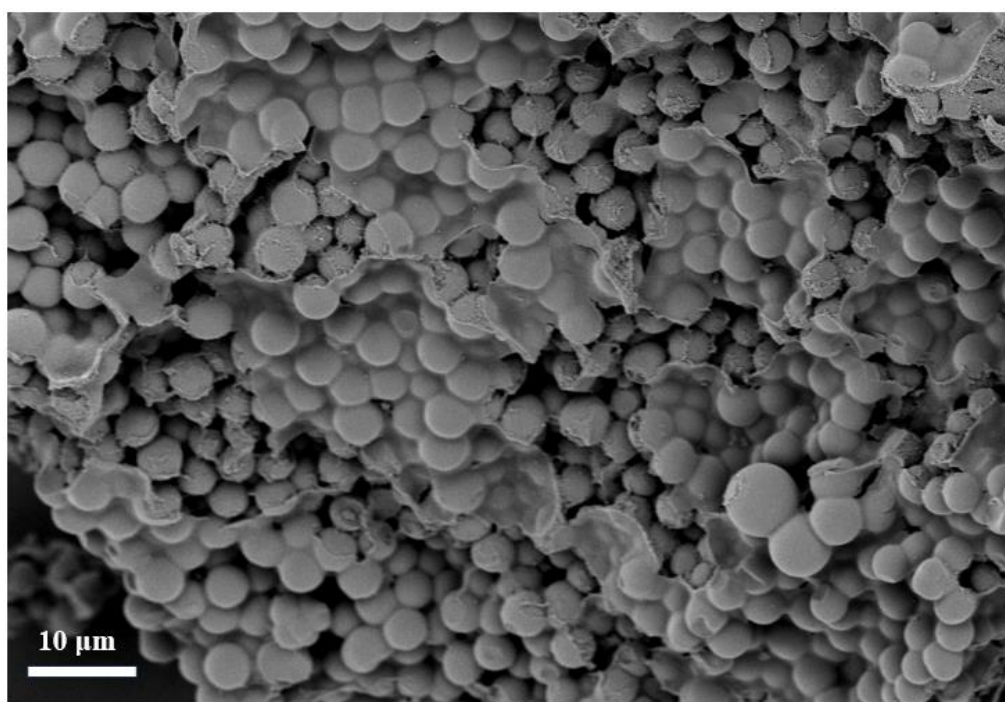


Figure S1. SEM image of the P@C.

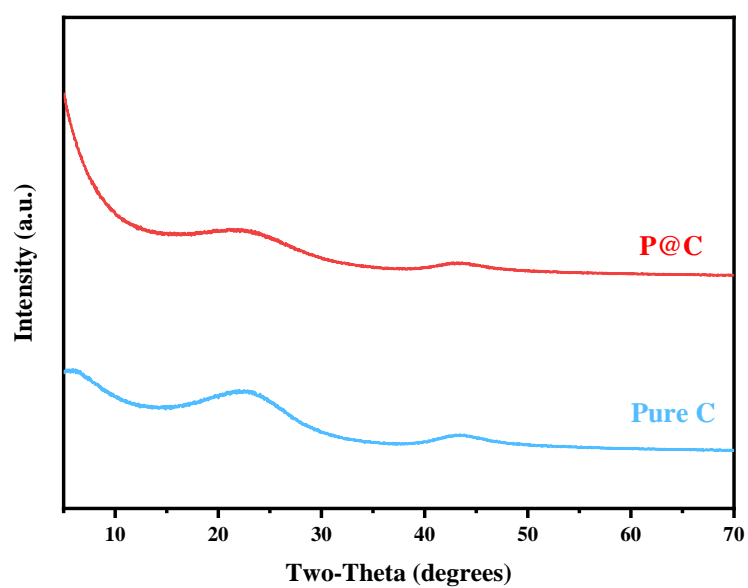


Figure S2. XRD pattern of the P@C and Pure C. Both samples show two typical diffraction peaks at 2θ of 24° and 44° which respectively corresponded to (002) plane and (100) plane.

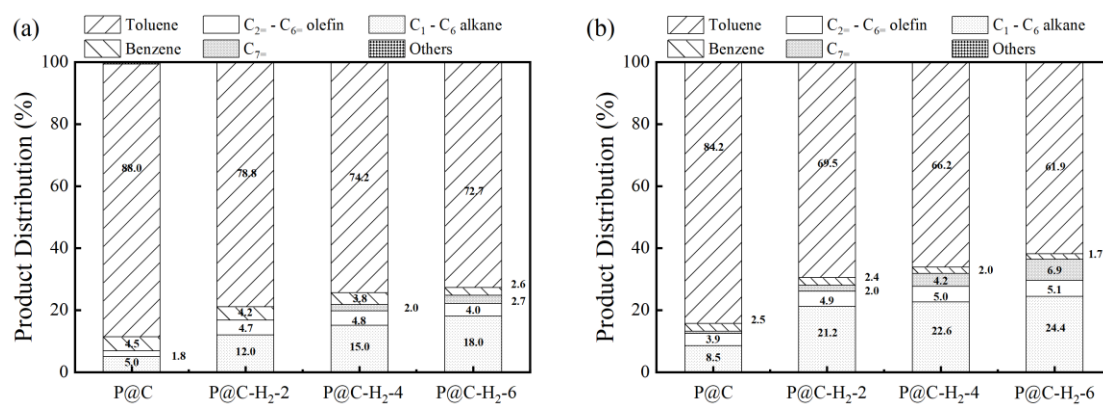


Figure S3. Comparison of products distribution (a) at 15 min and (b) at 260 min of P@C-H₂-x

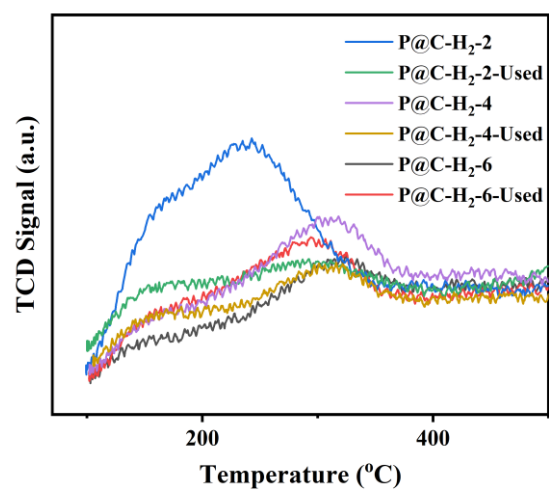


Figure S4. NH₃-TPD cruves of P@C-H₂-x-Used (x = 0, 2, 4, 6).

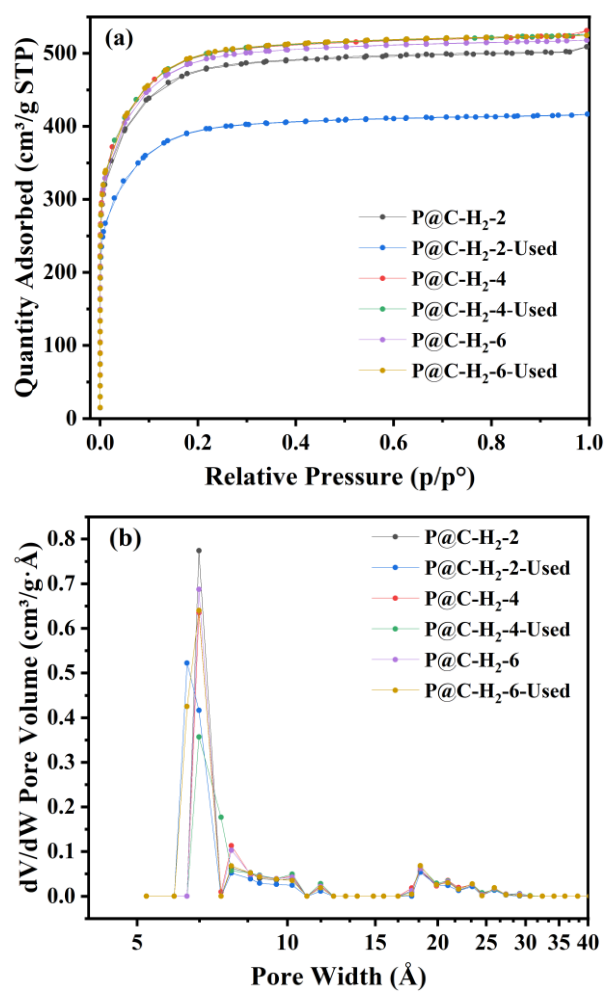


Figure S5. (a) N₂ sorption isotherms and (b) pore size distribution of P@C-H₂-x (x=0, 2, 4, 6)

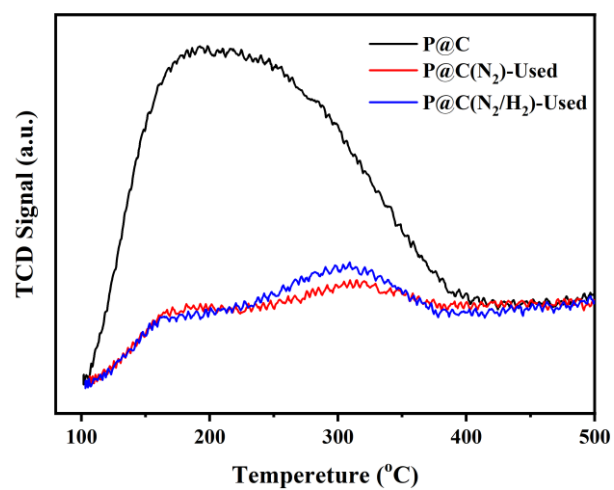


Figure S6. NH₃-TPD cruves of P@C in different H₂ concentration.

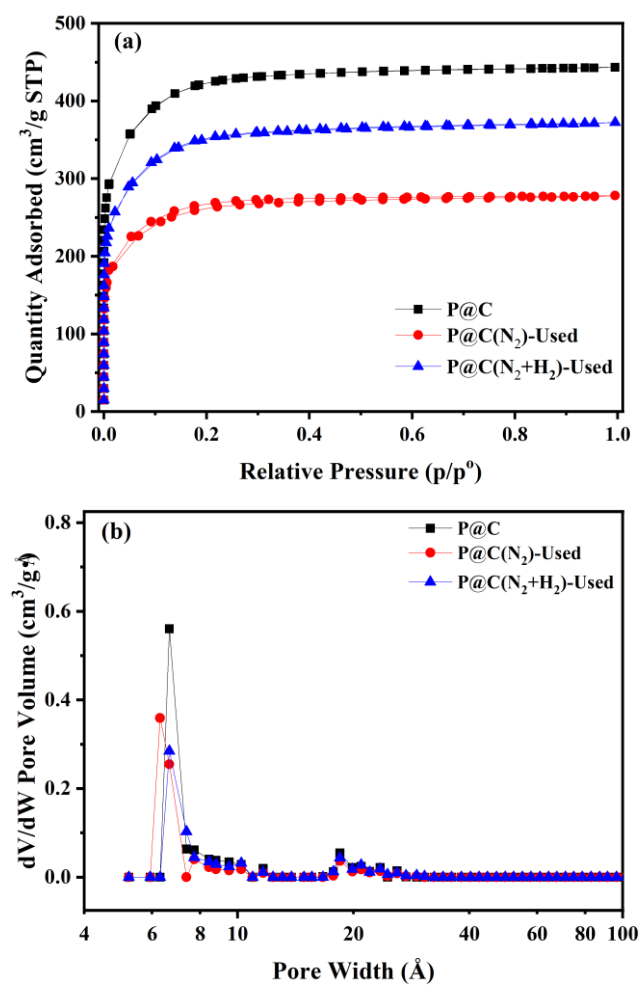


Figure S7. (a) N₂ sorption isotherms and (b) pore size distribution of P@C in different H₂ concentration

Table S1. The product distribution of P@C-H₂-x (x=0, 2, 4, 6) after 15 minutes of n-heptane dehydroaromatization.

Catalyst Selectivity (%)	P@C	P@C-H ₂ -2	P@C-H ₂ -4	P@C-H ₂ -6
Toluene	87.93	78.80	74.21	72.70
Benzene	4.52	4.23	3.84	2.56
C1	1.61	1.14	1.32	1.30
C2	1.27	2.24	2.56	3.18
C2=	0.39	0.23	0.28	0.34
C3	0.92	3.43	3.97	4.62
C3=	0.67	0.90	0.87	0.78
C4	0.84	3.33	4.43	5.05
C4=	0.69	1.81	1.75	1.33
C5	0.38	1.64	2.24	3.19
C5=	0.07	1.22	1.30	1.17
C6	0.02	0.24	0.51	0.69
C6=	0.02	0.54	0.56	0.43
C7=	0.00	0.07	1.99	2.66
Other	0.67	0.18	0.17	0.00

Table S2. Acidity and textual properties of P@C-H₂-x (x = 0, 2, 4, 6).

Sample	Total acidity ¹ ($\mu\text{mol g}^{-1}$)	S_{BET} ($\text{m}^2 \text{g}^{-1}$)	V_t ² ($\text{cm}^3 \text{g}^{-1}$)	D ³ (\AA)
P@C-Used	29.56	946.3	0.4302	5.49
P@C-H ₂ -2-Used	21.69	1422.2	0.6443	5.48
P@C-H ₂ -4-Used	20.67	1515.5	0.7402	5.51
P@C-H ₂ -6-Used	17.94	1592.5	0.7614	5.52

¹ Total acidity obtained by NH₃-TPD analysis; ² Volume calculated by the t-plot method; ³ Diameter calculated by Horvath-Kawazoe method; ⁴ Carbon deposition calculated by TG.