Supporting Information

Intermetallic $PdCu_3$ Supported on Nanodiamond-Graphene for Semi-hydrogenation of Phenylacetylene

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Experimental section

The TOF calculation methods were provided in supporting information.

$$TOF\ (h^{-1}) = \frac{rate\ of\ product\ formation\ (styrene)}{mole\ of\ active\ site} \qquad (1)$$

The Pd loading is used as the number of active sites in the TOF calculation process.

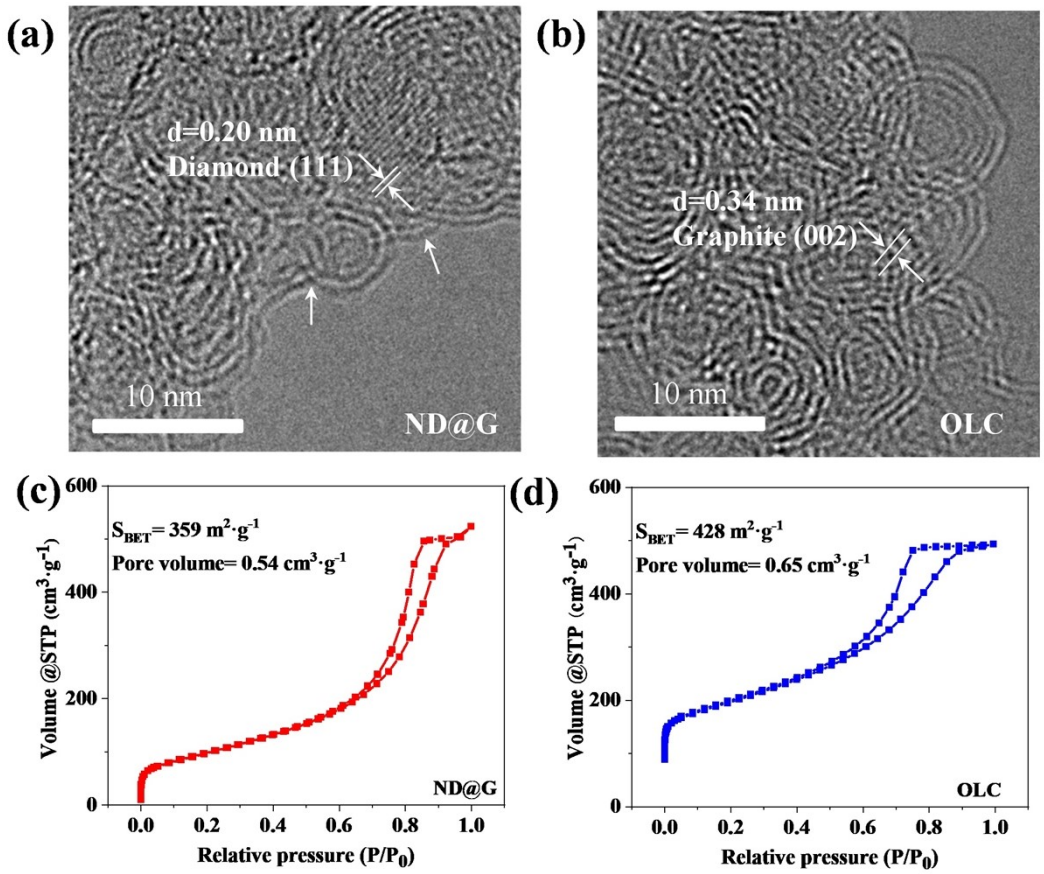

Figure S1. (a, b) HRTEM images of ND@G (a) and OLC (b). (c, d) Nitrogen adsorption-desorption isotherms of ND@G (c) and OLC (d).

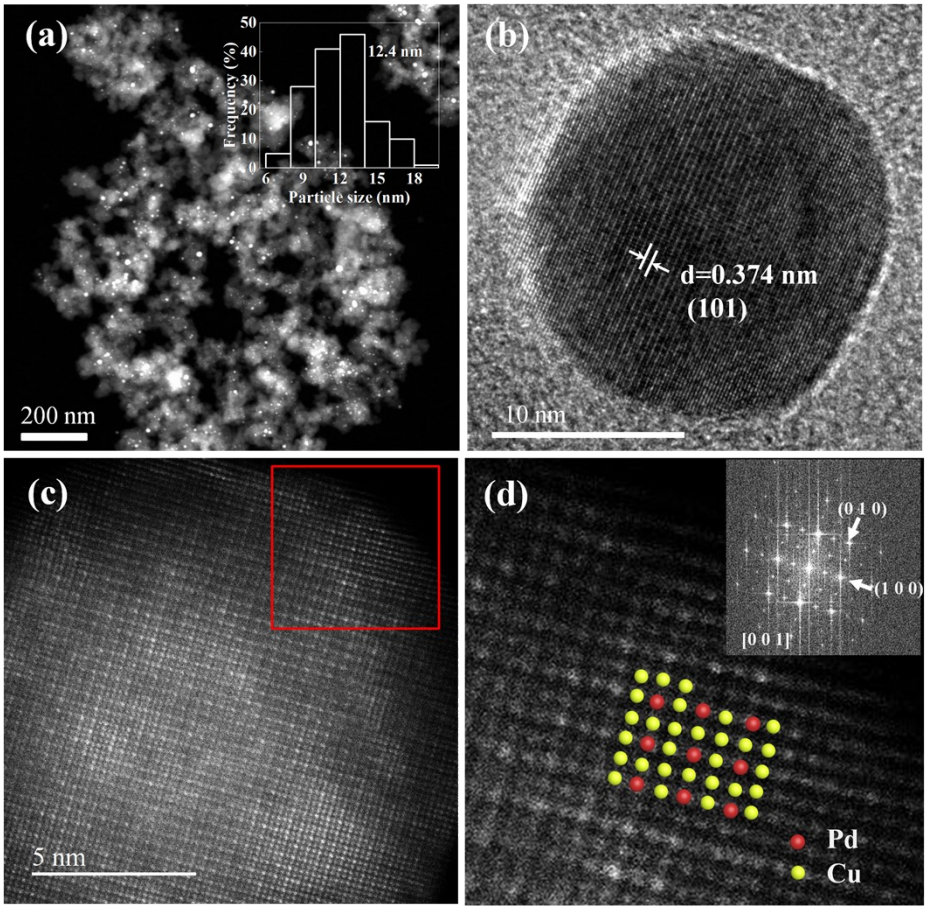

Figure S2. HADDF-STEM (a,c,d) and HRTEM (b) images of $PdCu_3$/ND@G; insets in a and d are the corresponding particle size distribution and the FFT pattern of $PdCu_3$/OLC.

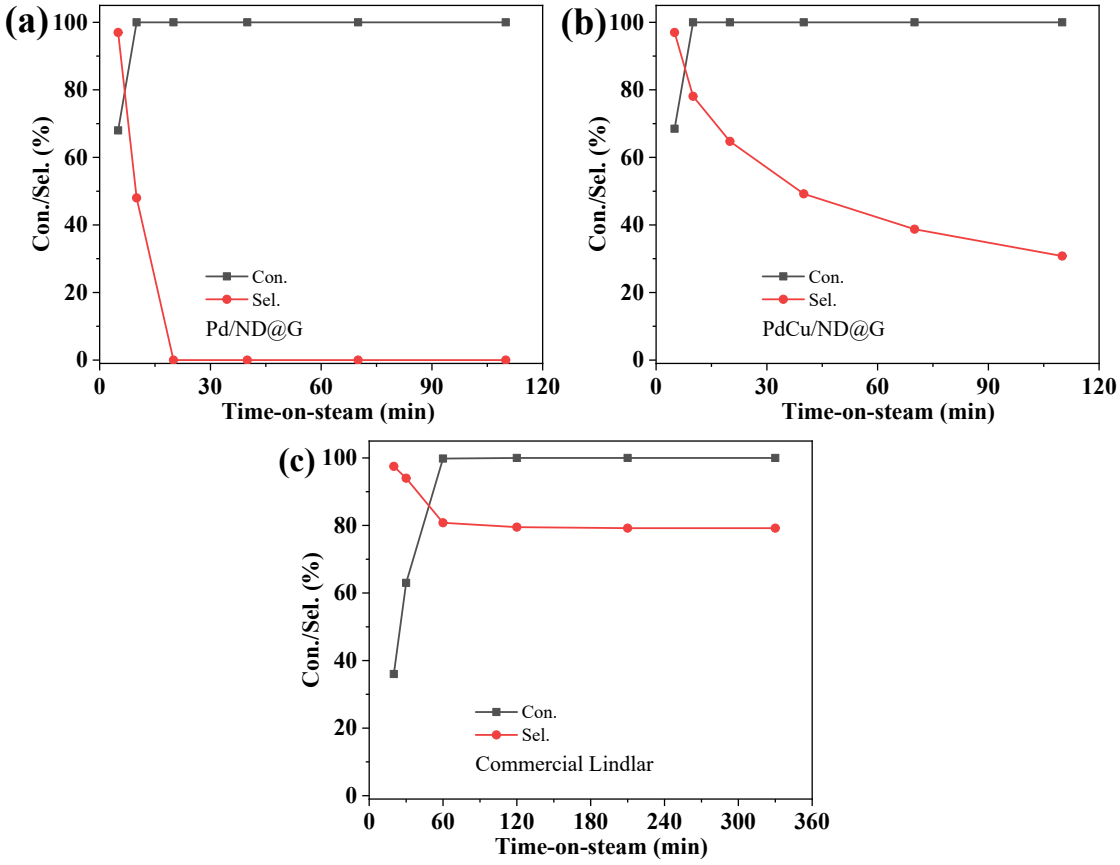

Figure S3. (a-c) Time-on-stream conversion and selectivity of phenylacetylene over Pd/ND@G (a), PdCu/ND@G (b), and commercial Lindlar catalysts (c).

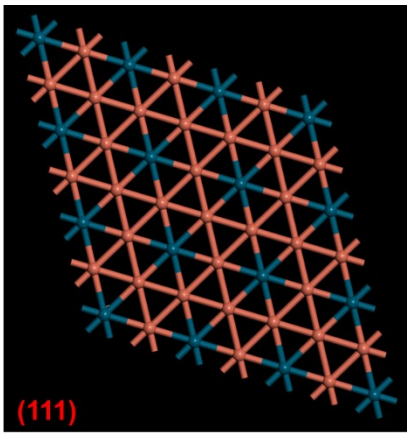

Figure S4. The (111) plane of intermetallic $PdCu_3$

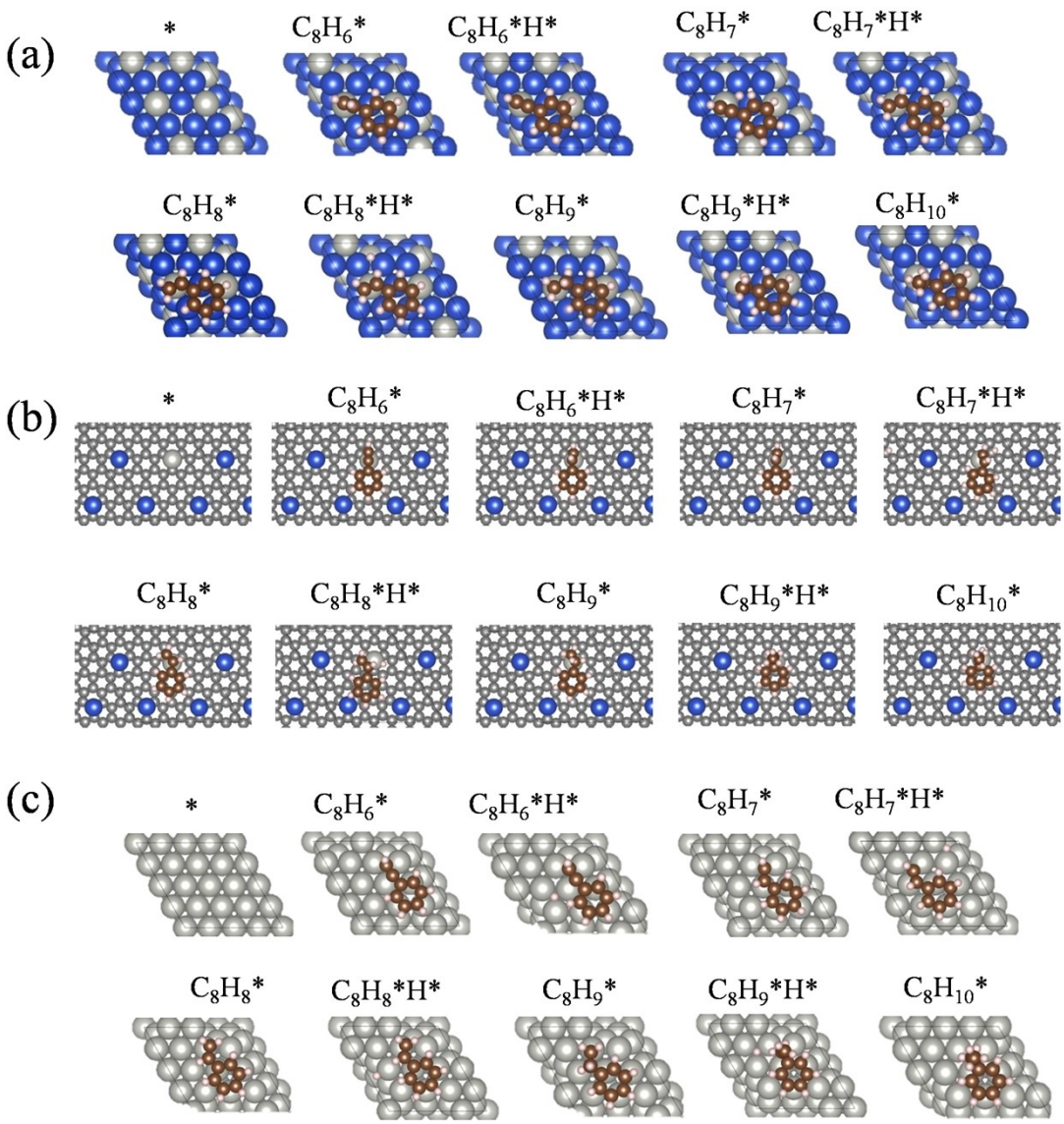

Figure S5. (a-c) Pictorial models for $PdCu_3$/OLC (a), $PdCu_3$/ND@G (b), and Pd (c), and their corresponding adsorption structure of C_8H_6*, C_8H_6*H, C_8H_7*, C_8H_7*H*, C_8H_8*, C_8H_8*H*, C_8H_9*, C_8H_9*H*, and C_8H_{10}*.

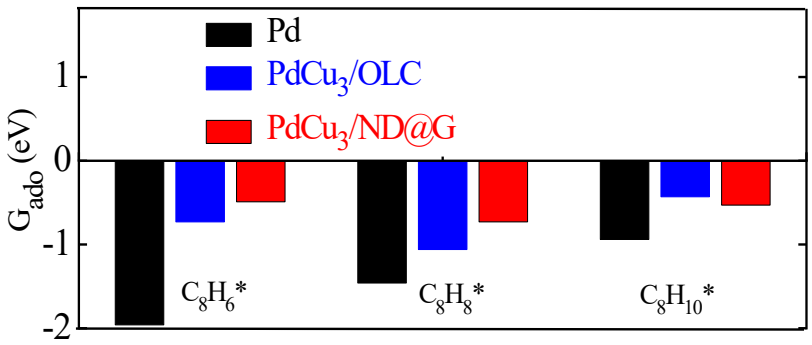

Figure S6. the adsorption energetics of C_8H_6* , C_8H_8* , and C_8H_{10}* on Pd, $PdCu_3$/OLC, and $PdCu_3$/ND@G.

Table S1. The change in Gibbs free energy for each elementary reaction.

ΔG	Pd	$PdCu_3$/OLC	$PdCu_3$/ND@G
ΔG_1	1.96	0.73	0.49
ΔG_2	0.28	0.15	0.55
ΔG_3	0.41	0.87	1.19
ΔG_4	0.46	0.04	0.31
ΔG_5	0.19	1.11	1.37
ΔG_{6a}	0.41	0.19	0.49
ΔG_{6b}	1.46	1.06	0.73
ΔG_7	0.27	0.01	0.3
ΔG_8	1.16	1.16	1.76
ΔG_9	1.42	1.63	2.67
ΔG_{10}	0.94	0.43	0.53