

Supporting Information

Controllable deposition of Bi onto Pd for selective hydrogenation of acetylene

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Table S1. ICP-OES analysis of Pd NCs@Bi_x.

Samples	Nominal ratio of Bi/Pd (mol%) ^a	Actual ratio of Bi/Pd (mol%) ^b
Pd NCs@Bi _{0.06}	0.06	0.06
Pd NCs@Bi _{0.25}	0.25	0.26
Pd NCs@Bi _{0.5}	0.50	0.47
Pd NCs@Bi ₁	1.00	1.02

^a Determined by the concentration of PdNCs and Bi precursors added.

^b Determined by ICP-OES analysis.

Table S2. ICP-OES analysis of catalysts.

Catalysts	Loading amount of Pd / wt%	Loading amount of Bi/ wt%
Pd NCs@Bi _{0.06} /Al ₂ O ₃	0.23	0.03
Pd NCs@Bi _{0.25} /Al ₂ O ₃	0.19	0.12
Pd NCs@Bi _{0.5} /Al ₂ O ₃	0.21	0.21
Pd NCs@Bi ₁ /Al ₂ O ₃	0.19	0.42
Pd _{7nm} NCs@Bi _{0.5} /Al ₂ O ₃	0.18	0.20
Pd _{7nm} NCs@Bi ₁ /Al ₂ O ₃	0.22	0.39
Pd _{7nm} NCs@Bi _{1.3} /Al ₂ O ₃	0.19	0.50
Pd NPs@Bi ₁ /Al ₂ O ₃	0.18	0.38
Pd NPs@Bi _{0.8} /CaCO ₃	0.22	0.29

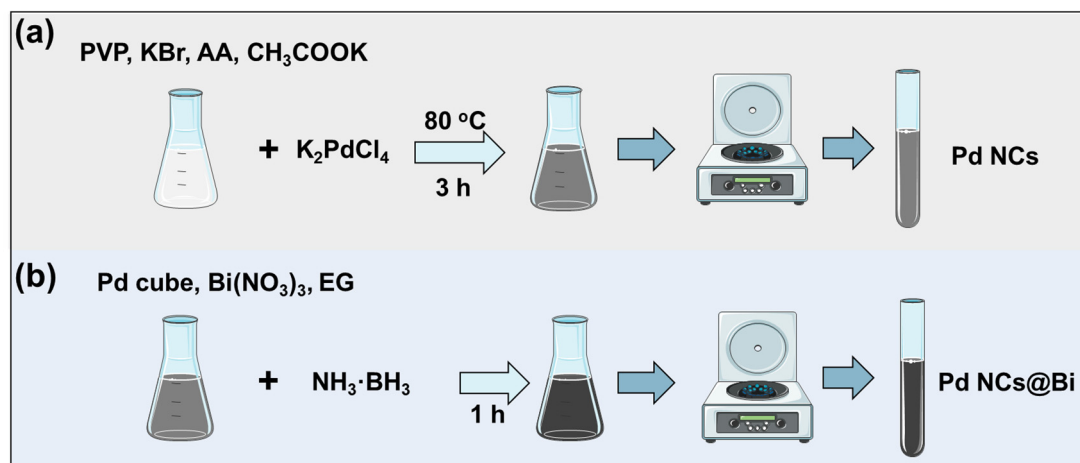


Figure S1. Schematic illustration of (a) Pd nanocubes (Pd NCs) and (b) site-specific deposition of Bi on Pd nanocubes (Pd NCs@Bi) synthesis.

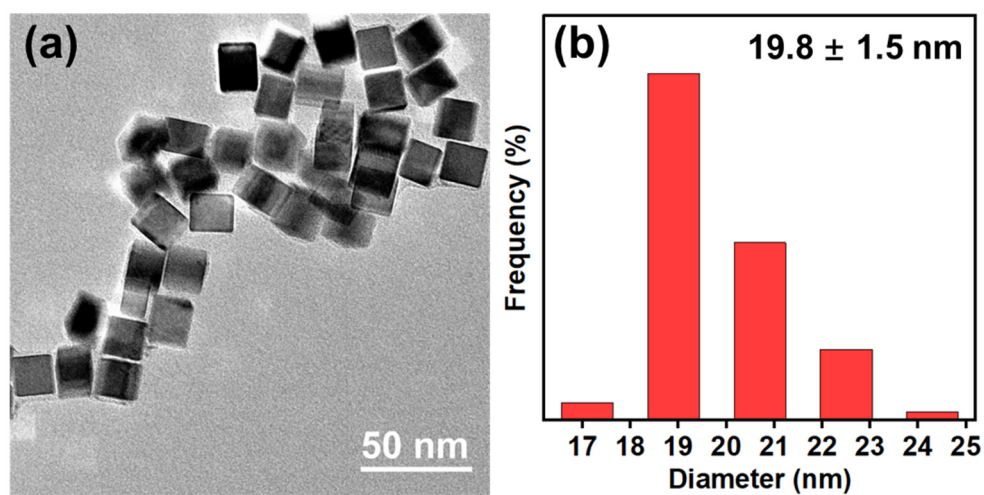


Figure S2. (a) HRTEM image and (b) size distribution of 20 nm sized Pd NCs.

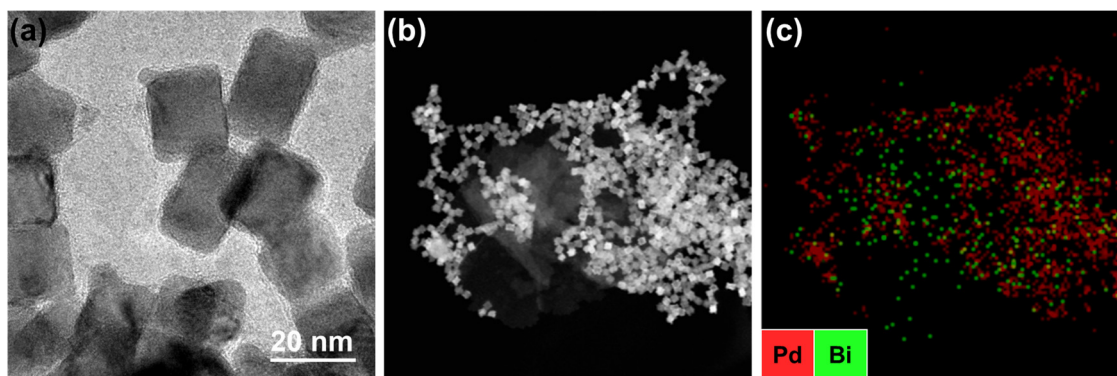


Figure S3. (a) HRTEM image and (b-c) EDS elemental maps of Pd NCs@Bi_{0.25} using NaBH₄ as reductant.

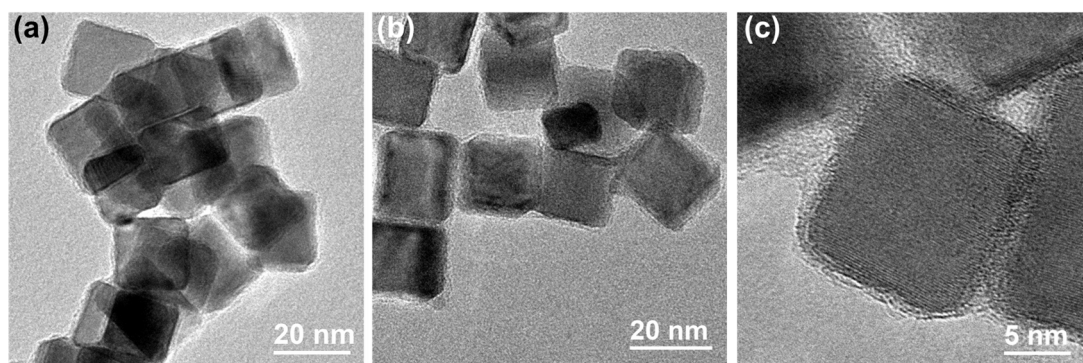


Figure S4. HRTEM images of Pd NCs@Bi_{0.25} using NH₃·BH₃-NaOH as reductant.

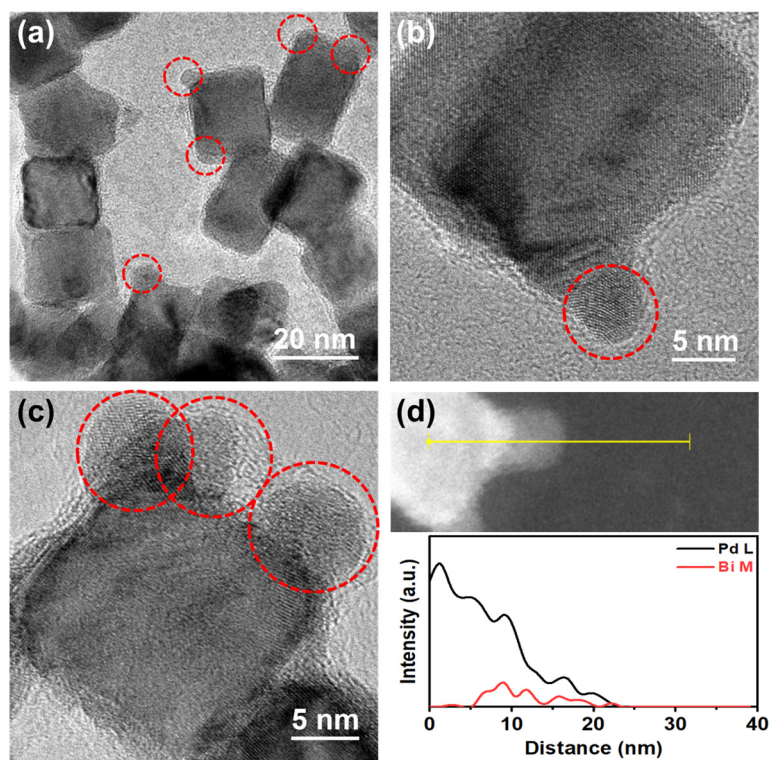


Figure S5. (a-c) HRTEM images and (d) line scanning profile of Pd NCs@Bi_{0.06}.

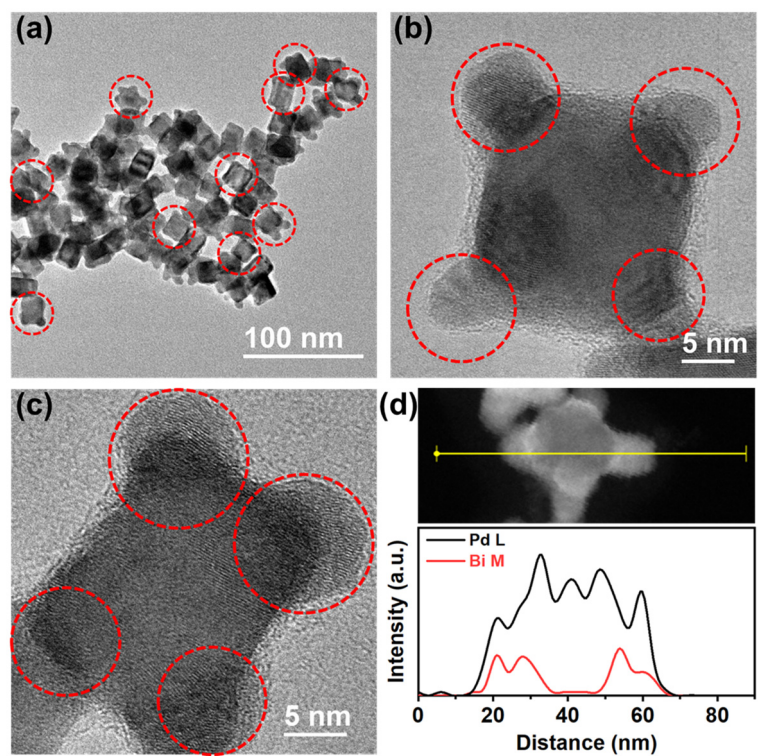


Figure S6. (a-c) HRTEM images and (d) line scanning profile of Pd NCs@Bi_{0.25}.

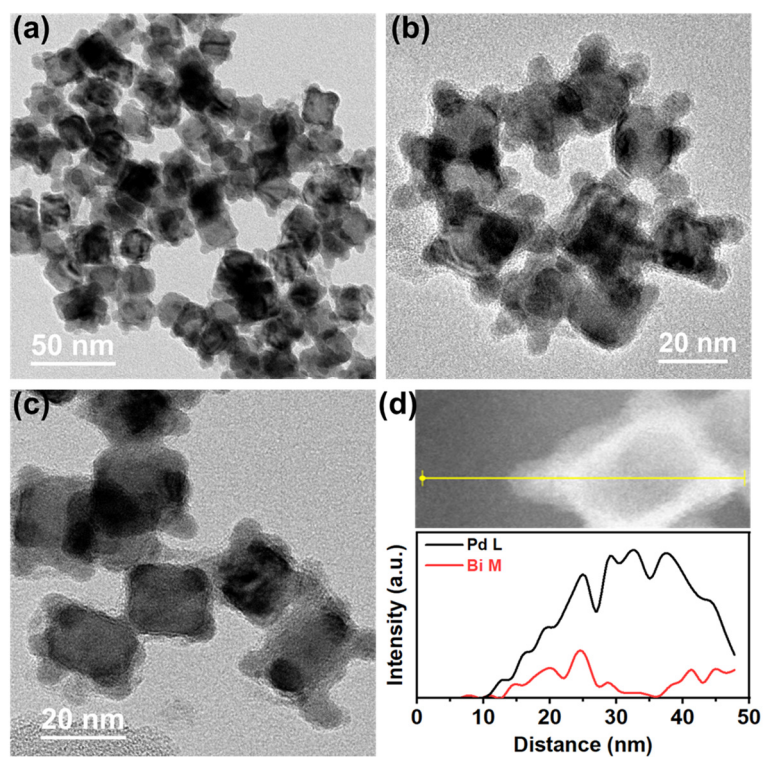


Figure S7. (a-c) HRTEM images and (d) line scanning profile of Pd NCs@Bi_{0.5}.

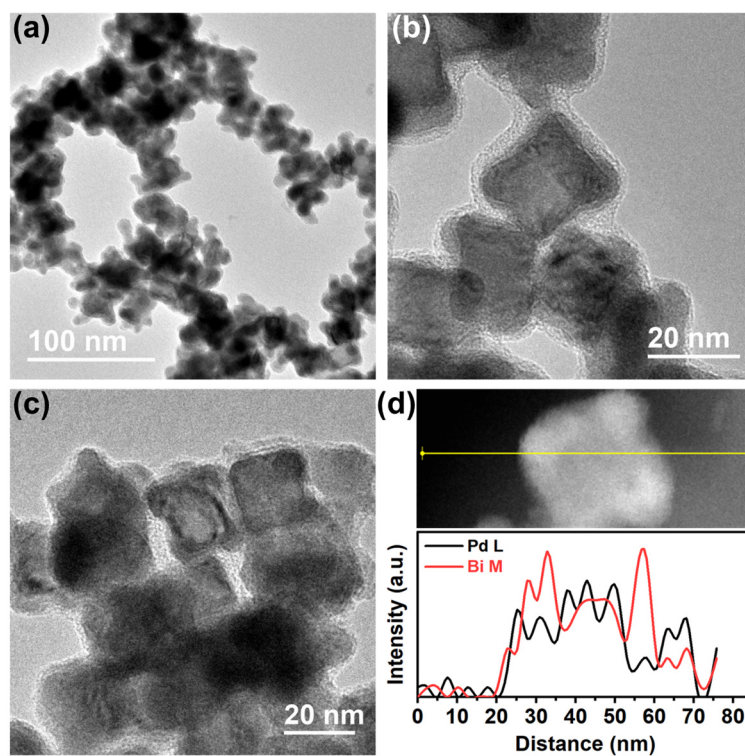


Figure S8. (a-c) HRTEM images and (d) line scanning profile of Pd NCs@Bi₁.

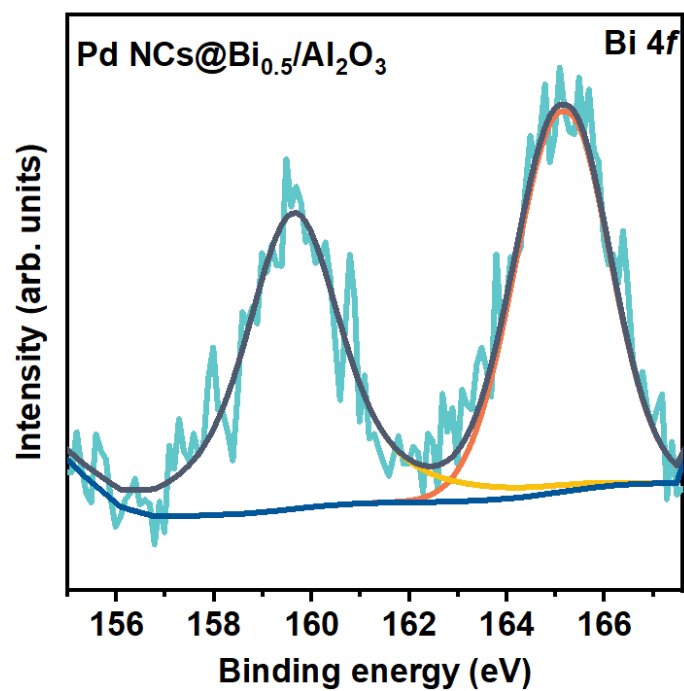


Figure S9. Bi 4f XPS spectra of Pd NCs@Bi_{0.5}/Al₂O₃ catalyst. Notably, Pd 3d signal was undetectable due to the low Pd content (0.2 wt.%) and the fact that Bi coating on the surface of the Pd NCs could affect the signal of Pd.

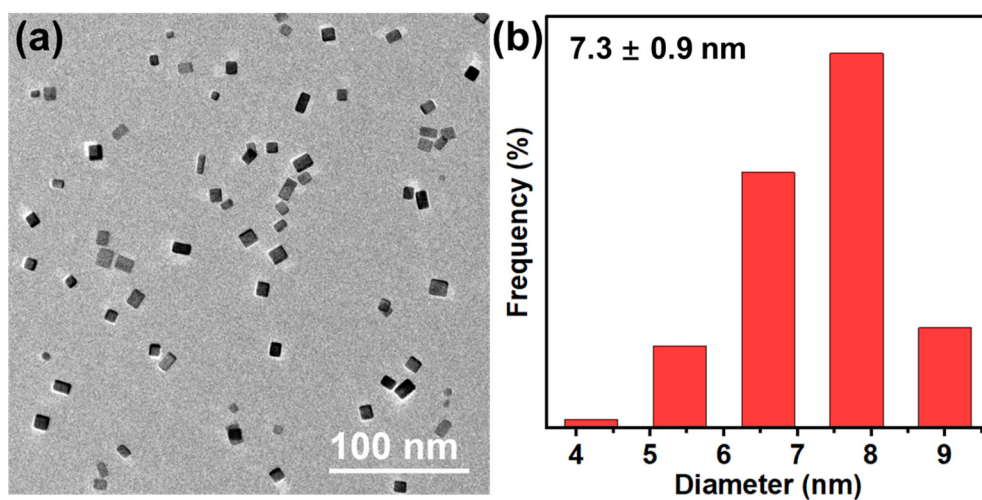


Figure S10. (a) HRTEM image and (b) size distribution of 7 nm sized Pd NCs.

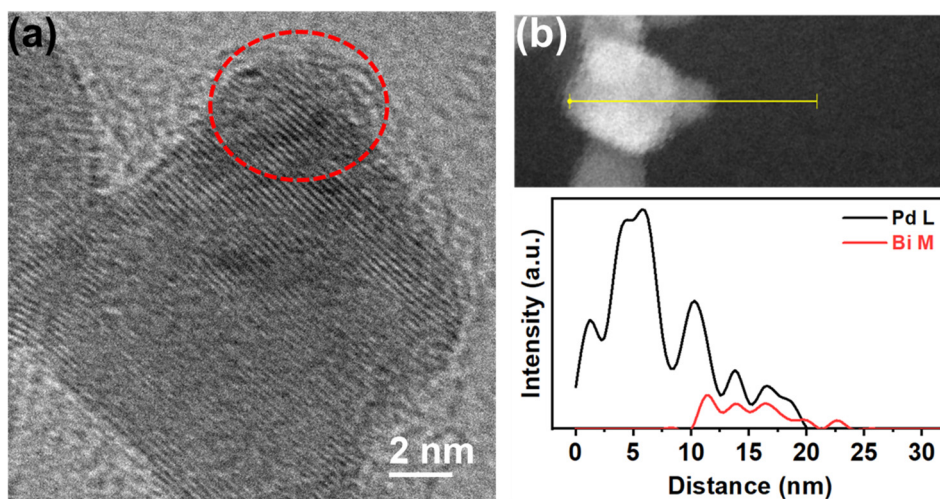


Figure S11. (a) HRTEM images and (b) line scanning profile of Pd_{7nm} NCs@Bi_{0.5}.

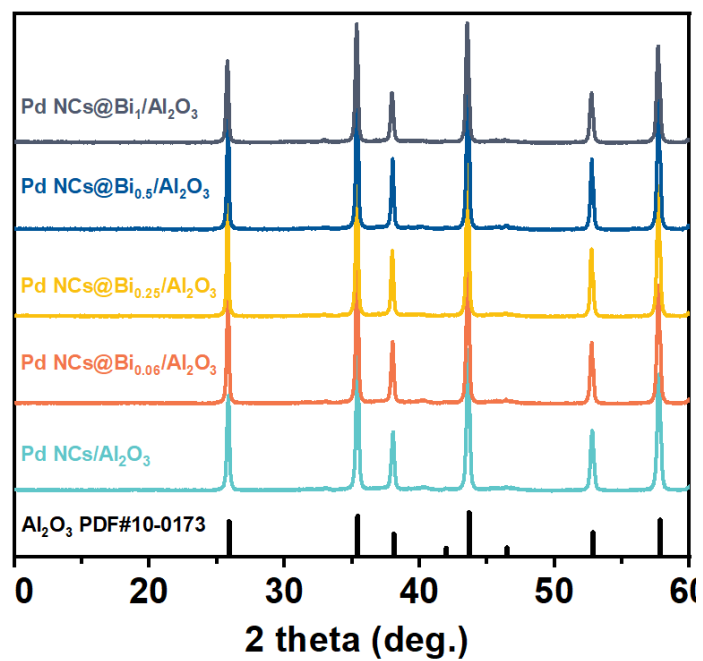


Figure S12. XRD patterns of Pd NCs/Al₂O₃, Pd NCs@Bi_{0.06}/Al₂O₃, Pd NCs@Bi_{0.25}/Al₂O₃, Pd NCs@Bi_{0.5}/Al₂O₃ and Pd NCs@Bi₁/Al₂O₃ catalysts.

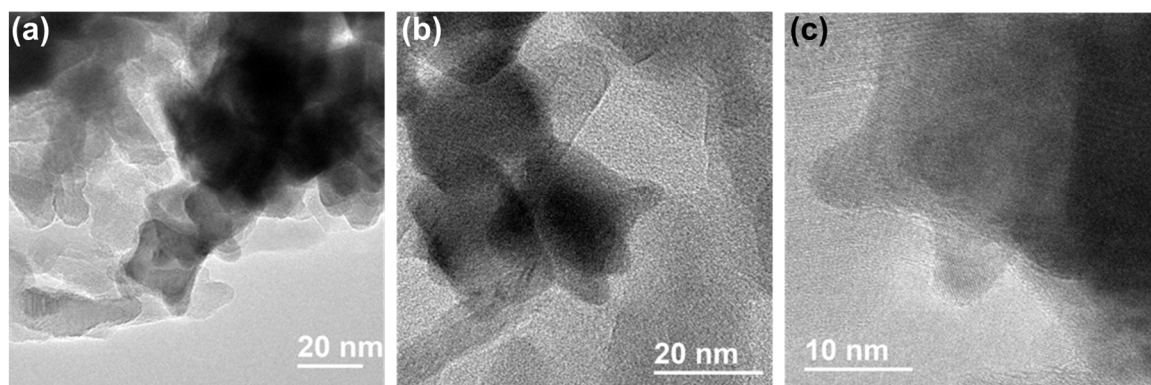


Figure S13. HRTEM images of Pd NCs@Bi_{0.5}/Al₂O₃-spent catalyst.

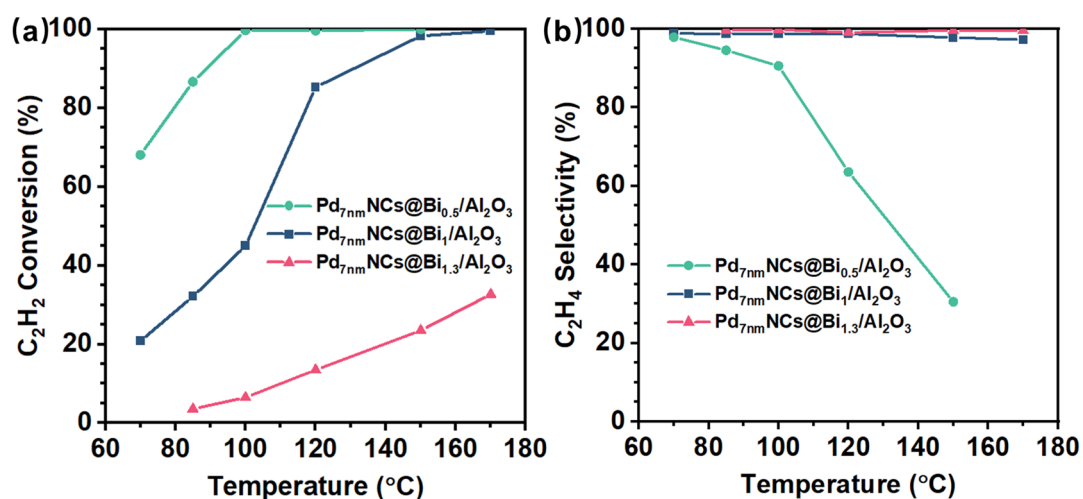


Figure S14 Catalytic performances of $\text{Pd}_{7\text{nm}}\text{NCs}@Bi_x/Al_2O_3$ catalysts in acetylene hydrogenation. (a) C_2H_2 conversion as a function of reaction temperature and (b) C_2H_4 selectivity as a function of reaction temperature. (Reaction conditions: space velocity of $120000\text{ mL h}^{-1}\text{ g}^{-1}$ and reactant gases: 1.0 vol % C_2H_2 , 20.0 vol % C_2H_4 , 20.0 vol % H_2 , and 59 vol % N_2).

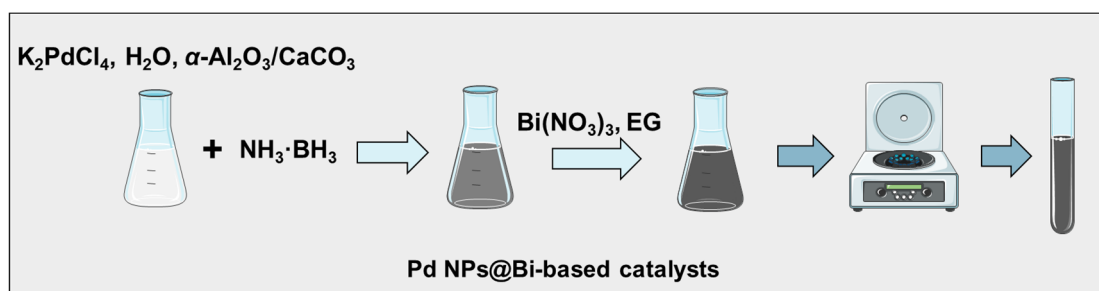


Figure S15. Schematic illustration of Pd NPs@Bi-based catalysts synthesis.

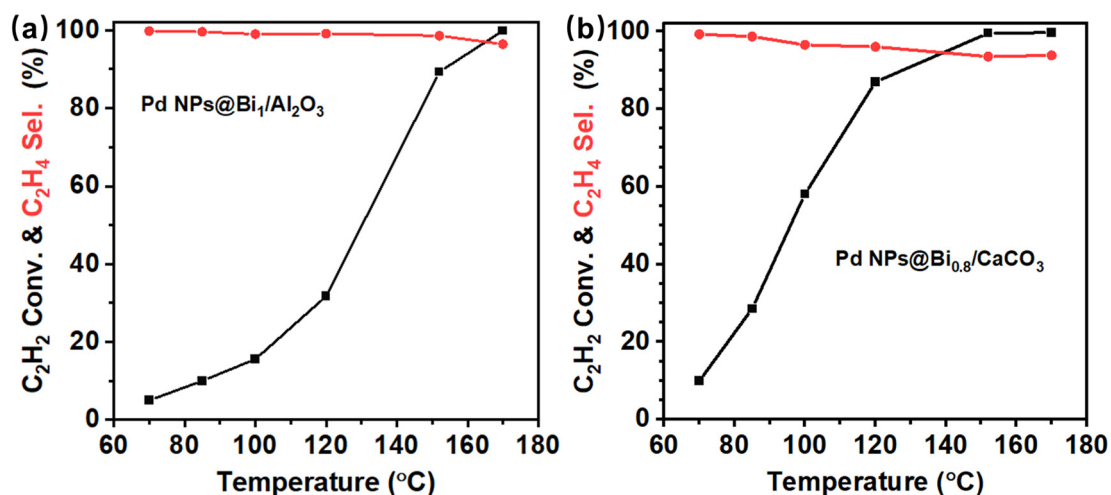


Figure S16 Catalytic performances of Pd NPs@Bi based catalysts in acetylene hydrogenation. (a) C₂H₂ conversion and C₂H₄ selectivity as a function of reaction temperature over Pd NP@Bi₁/Al₂O₃ and (b) C₂H₂ conversion and C₂H₄ selectivity as a function of reaction temperature over Pd NP@Bi_{0.8}/CaCO₃. (Reaction conditions: space velocity of 120000 mL h⁻¹ g⁻¹ and reactant gases: 1.0 vol % C₂H₂, 20.0 vol % C₂H₄, 20.0 vol % H₂, and 59 vol % N₂).