Electronic Supplementary Material (ESI) for Green Chemistry.

Ru Single Atoms for Efficient Chemoselective Hydrogenation of Nitrobenzene to Azoxybenzene

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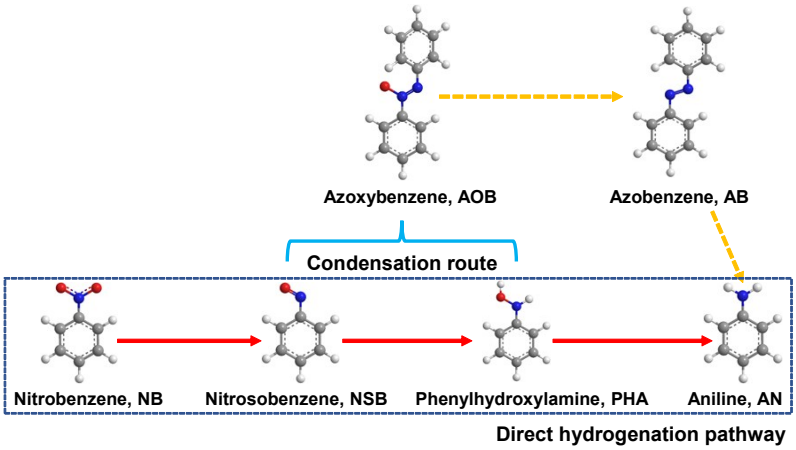
The supporting information including

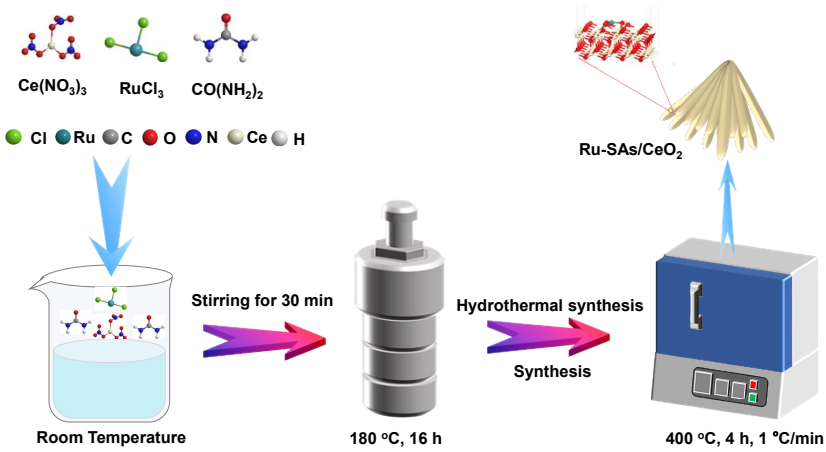
Scheme S1-S2

Table S1

Figure S1-S7



Scheme S1. Schematic illustrations of reaction pathway for nitrobenzene hydrogenation reaction, with C in gray, O in red, N in blue and H in white.



Scheme S2. Schematic illustrations of the preparation of Ru-SAs/CeO_2 catalyst, with C in gray, O in red, N in blue, H in white, Ru in teal, Ce in yellow, Cl in green.

Table S1. Element analysis and texture properties of various samples.

Entry	Catalysts	Ru loading [wt%]	S_{BET} [b] [m^2/g]	V_p [b] [cm^3/g]	Pore size [b] [nm]
1	CeO_2	0	53.9	0.08	6.2
2	Ru-SAs/CeO_2	1.6	88.2	0.09	3.9
3	Ru-NPs/CeO_2	1.7	51.8	0.06	4.3

[a]The concentration of Ru was measured by ICP-OES.

[b]Determined by N_2 adsorption/desorption isotherms.

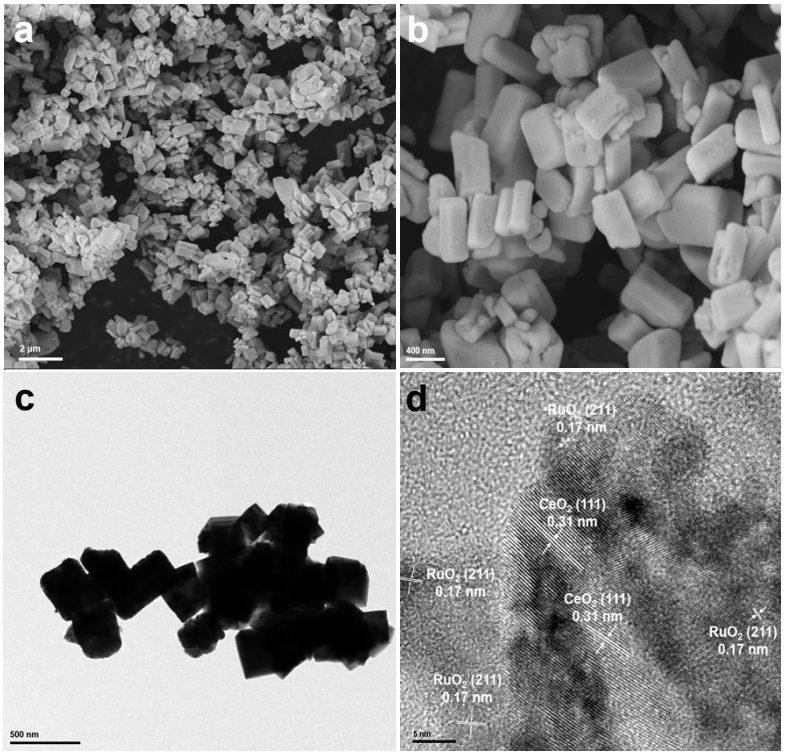


Figure S1. (a, b) SEM images. (c) TEM image, (d) Representative HRTEM image of the Ru-NPs/CeO_2.

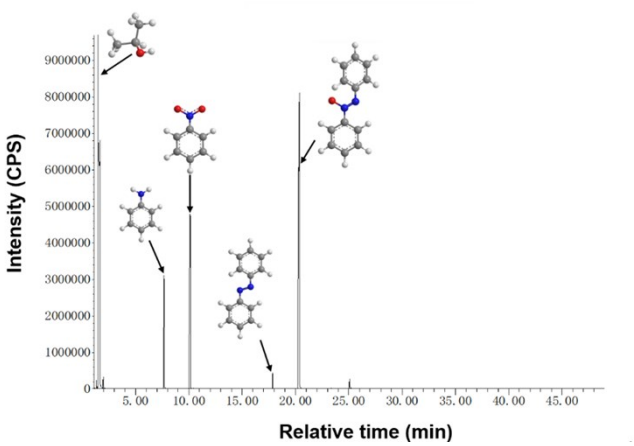


Figure S2. GC-MS spectrum of Ru-SAs/CeO_2 for the selective hydrogenation of nitrobenzene. Azoxybenzene was the main product, partial of aniline and trace azobenzene were also detected.

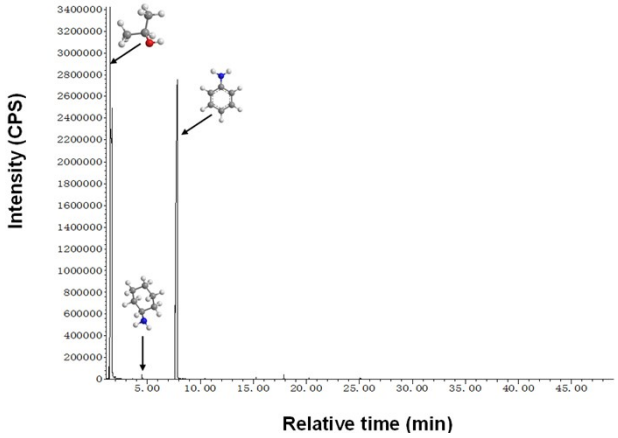


Figure S3. GC-MS spectrum of Ru-NPs/CeO_2 for the selective hydrogenation of nitrobenzene. Aniline was the main product, and trace cyclohexylamine was also detected.

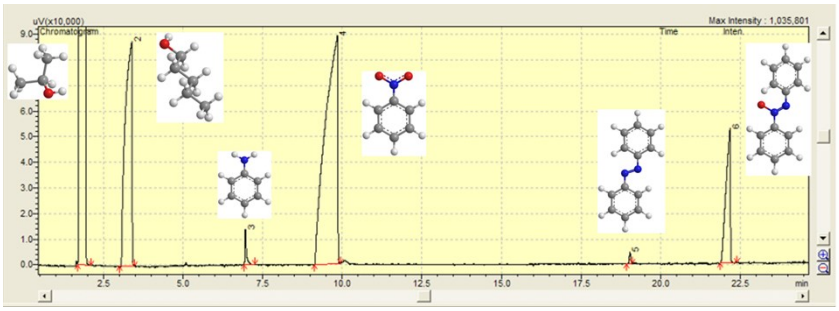


Figure S4. GC spectrum of Ru-SAs/CeO_2 for the selective hydrogenation of nitrobenzene. Azoxybenzene was the main product, and small proportion of aniline and azobenzene were also detected.

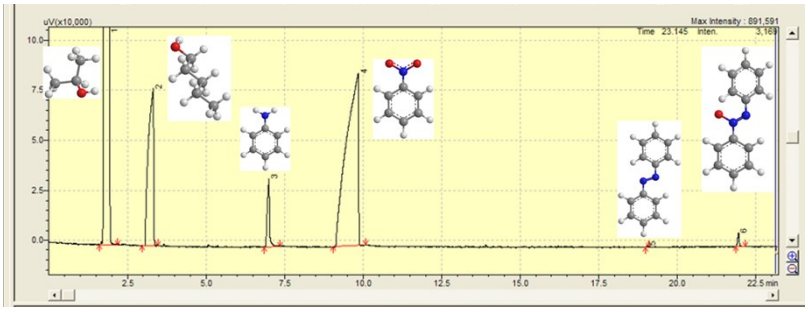


Figure S5. GC spectrum of Ru-NPs/CeO_2 for the selective hydrogenation of nitrobenzene. Aniline was the main product, small part of azobenzene and azoxybenzene were also detected.

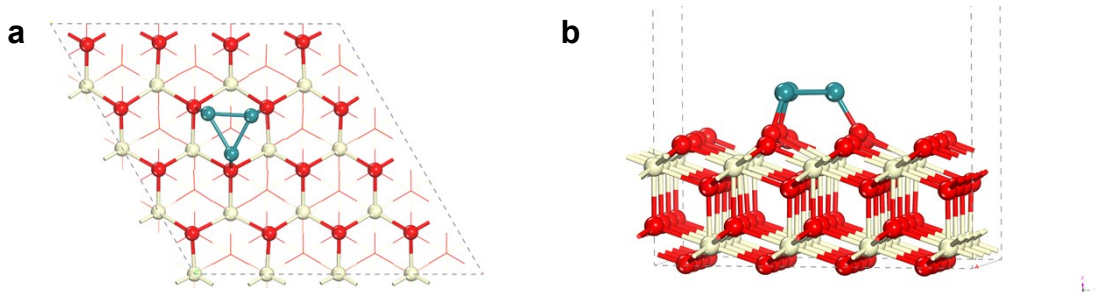


Figure S6. Coordinated structure of Ru_3 on the Ru-SCs/CeO_2 (111) surface. Top (a) and side (b) view of the detailed structure of Ru-SCs/CeO_2.

For the Ru-SCs/CeO_2 (111) structure, each Ru atom from the Ru_3 cluster was bonded with a surface lattice oxygen, with the Ru-O length was calculated to be 1.86 ~ 1.90 Å, with O in red, Ce in yellow and Ru in teal.

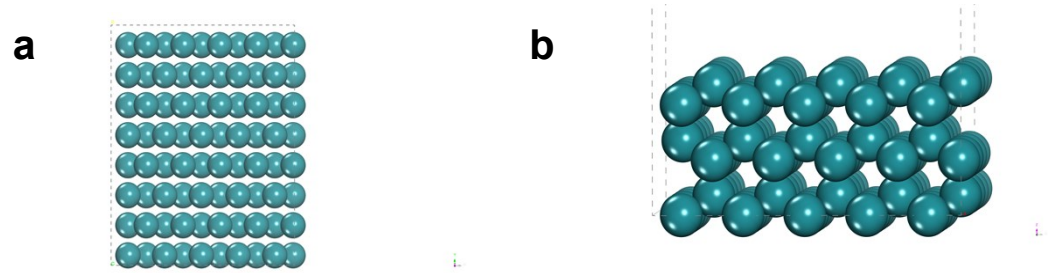


Figure S7. Top (a) and side (b) view of the detailed structure of metallic Ru (100) structure, with Ru in teal.