

Electronic Supplementary Information

Highly Efficient Hydrogenation of Nitroarenes by Co Nanoparticles Encapsulated in N-doped Carbon Nanotubes under Mild Conditions

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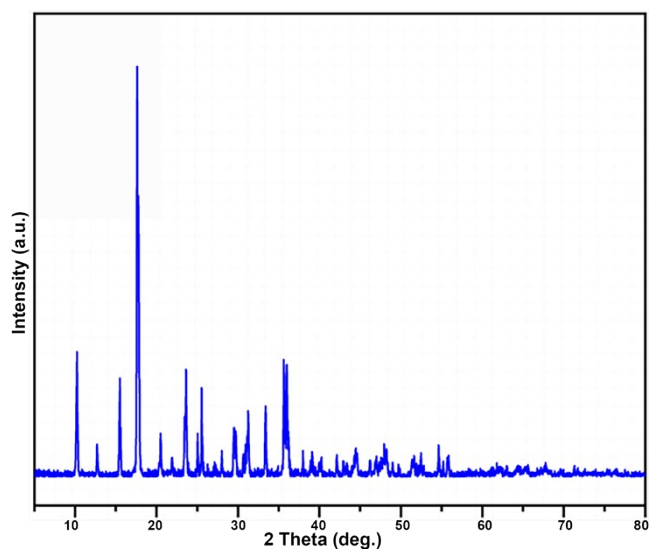


Figure S1. The PXRD of as-synthesized ahnu-11.

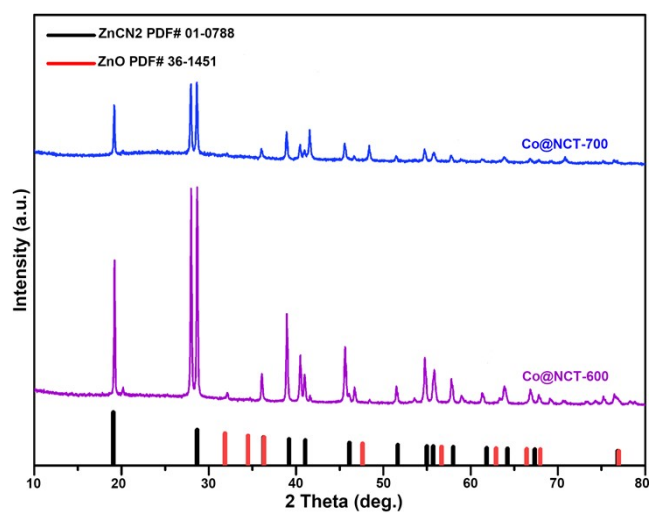


Figure S2. The PXRD of as-synthesized catalysts in a pyrolytic temperature range of 600-700°C.

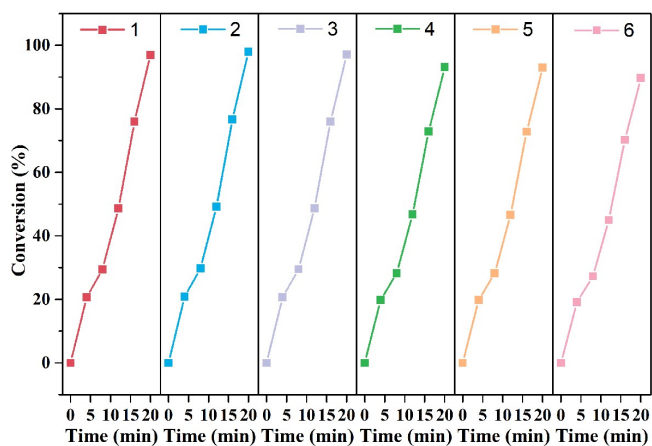


Figure S3. The catalytic performance of the cyclic hydrogenation of 4-nitrobenzene with Co@NCT-800 as catalyst.

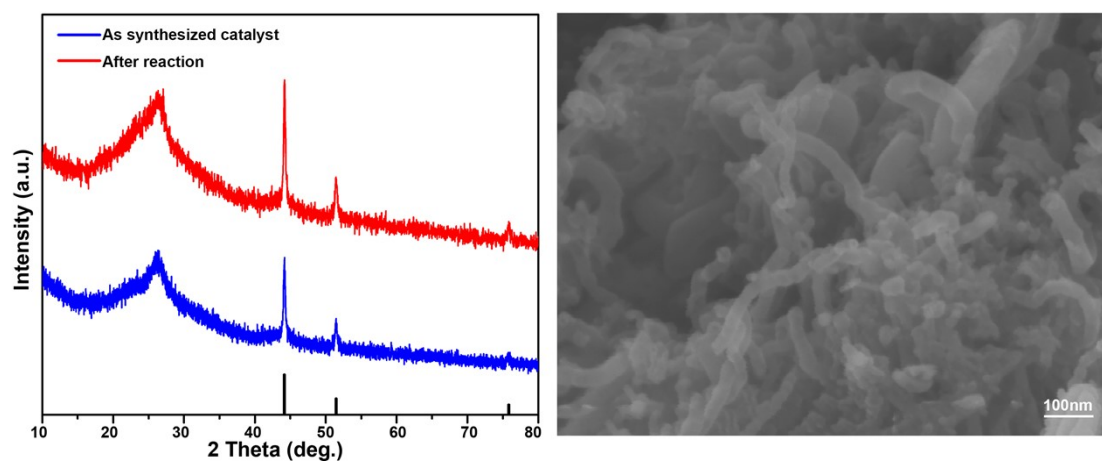


Figure S4. (Left) the XRD of as-synthesized and recycled Co@NCT-800; (Right) the SEM image of Co@NCT-800 after catalytic reactions.

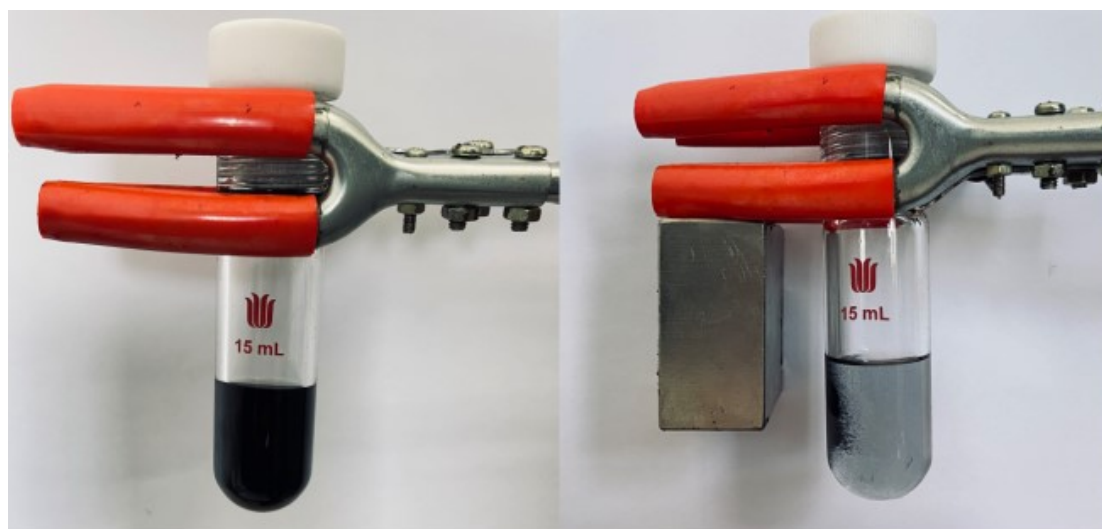
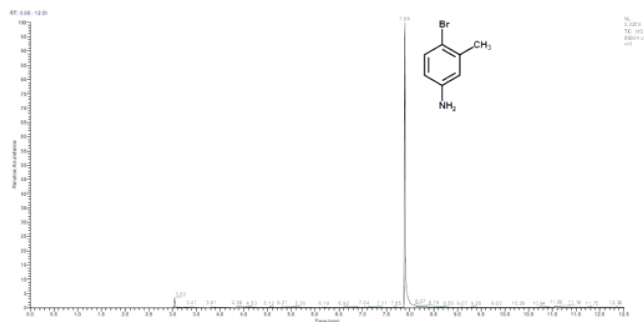
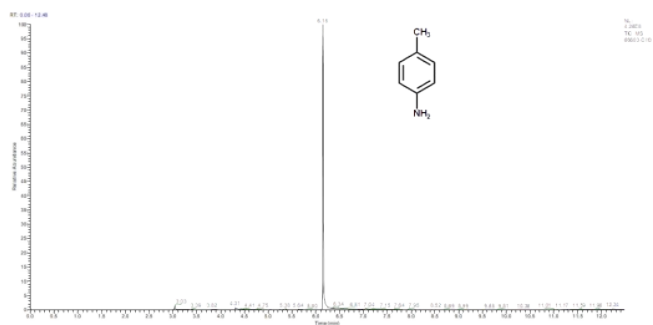
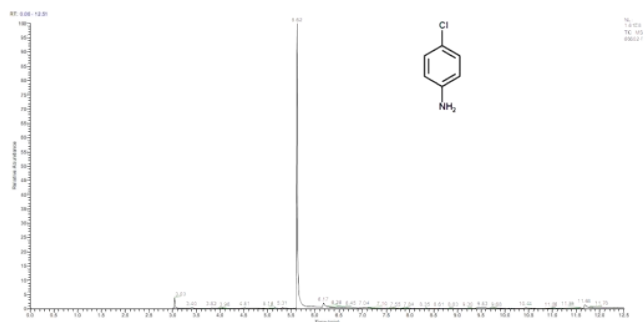
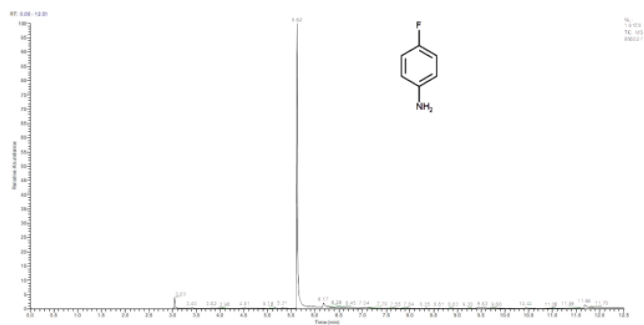
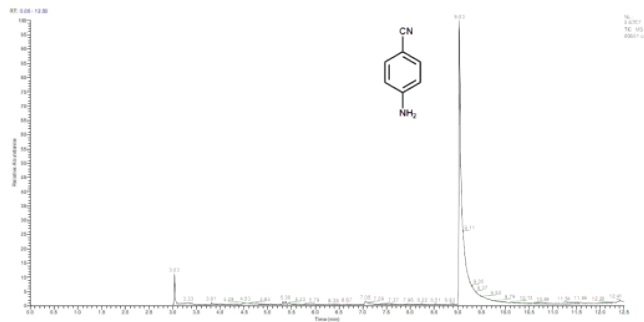


Figure S5. The Co@NCT-800 catalyst is easy to recover owing to its inherent magnetism (left and right: without and with an external magnet for the catalytic reaction system).



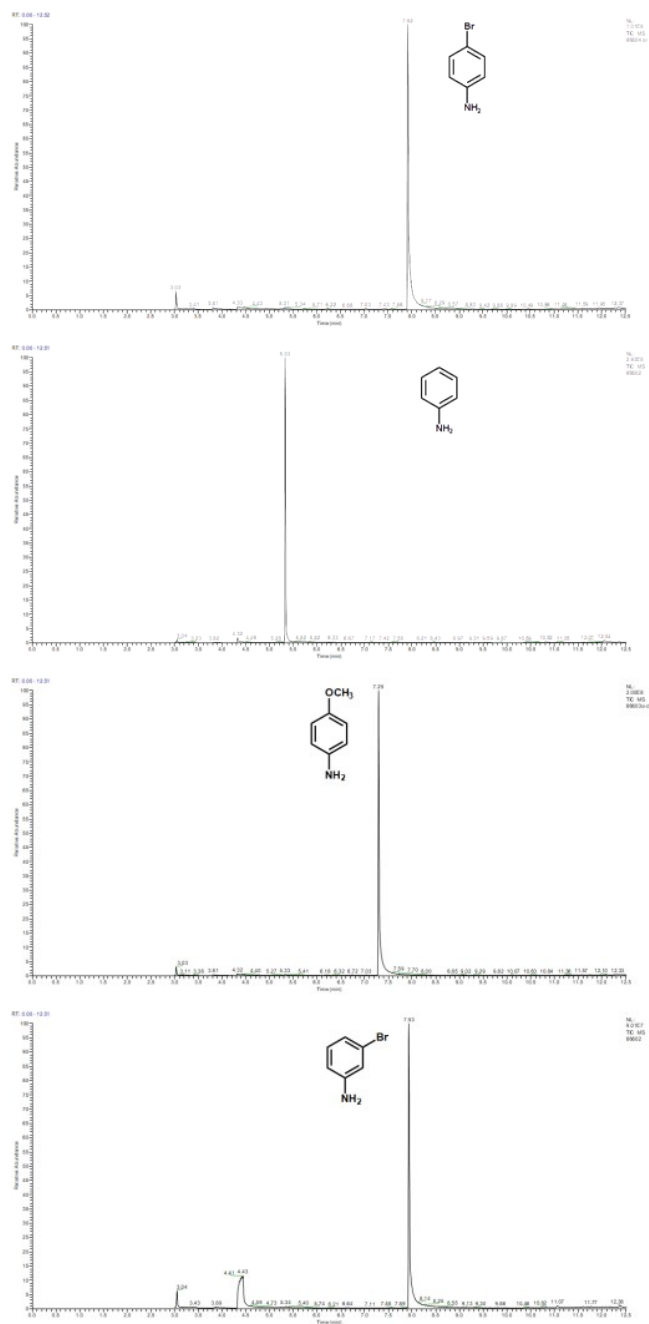


Figure S6. The GC spectra of nitro compounds after hydrogenation.

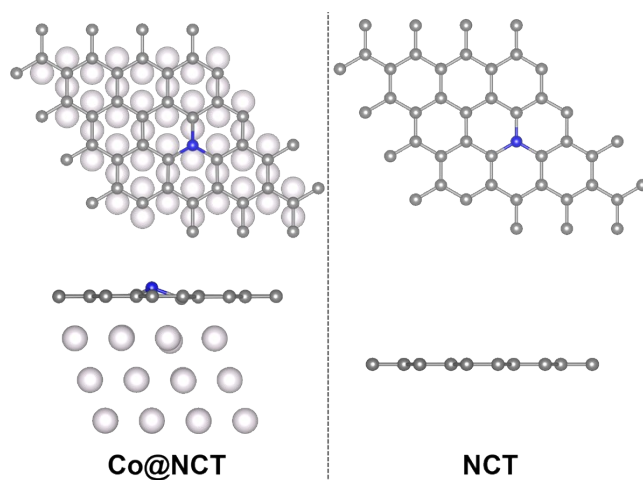


Figure S7. Top and side views of the most stable geometries of Co@NCT and NCT.

Table S1. Comparison of the catalytic activity of Co@NCT to recent reported Co-based catalysts in the hydrogenation of nitrobenzene to aniline.

Entry	Catalysts	T/°C	P/MPa	S/%	C/%	Reference
1	Co@NCT-800	40	0.1	>99	>99	This
2	Co SAs/NC	110	3	>99	59	[20]
3	Co@NMC-800	80	1	>99	>99	[42]
4	Co@N-doped carbon	110	5	>99	>99	[43]

Table S2. ICP-AES element analysis results for the materials.

Sample	The content of Zn (%)	The content of Co (%)
Co@NCT-600	17.1	7.2
Co@NCT-700	10.2	9.7
Co@NCT-800	0	14.7
Co@NCT-900	0	15.6

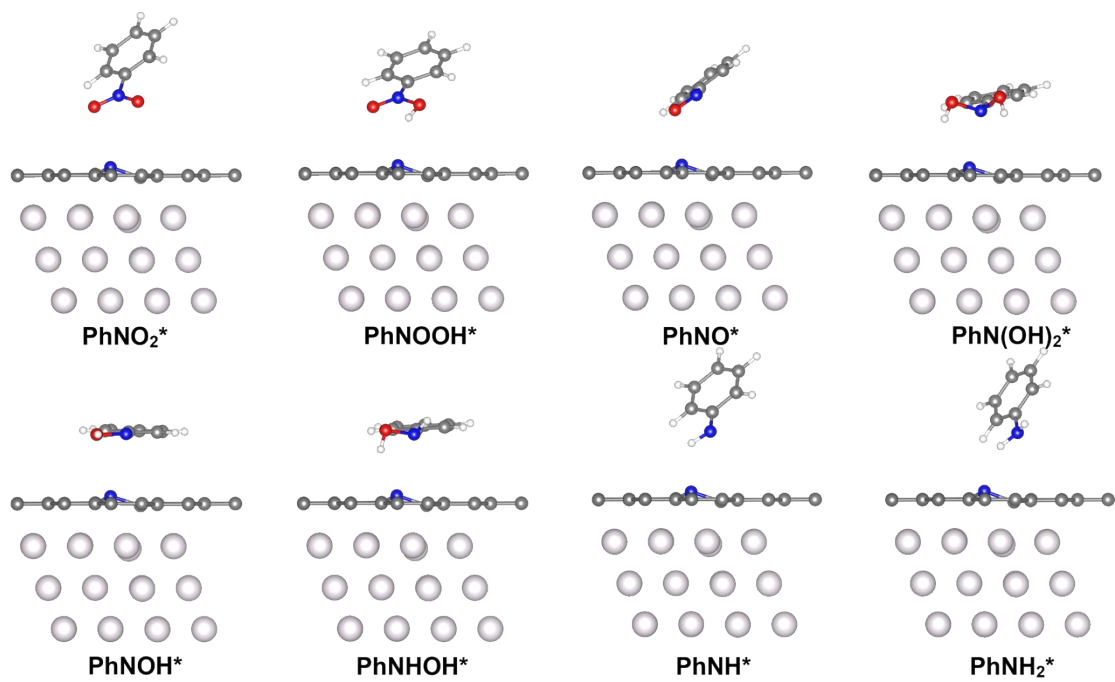


Figure S8. The optimized configuration of catalyst and reaction intermediates.

POSCAR for Co@NCT

Co C N

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-5.0119500160000001	8.6809520727000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.2686004639000004

Co C N

48 31 1

Selective Dynamics

Cartesian

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0.5497106627190300	3.4225520686922293	3.1691926849334271	T T T
0.5161807070880899	0.5254580202795790	5.1414929675683307	T T T
1.7965334631873997	4.1435052511823409	1.2500375407822586	F F F
1.7904691239548400	1.2611687518456642	3.1570373280769526	T T T
-0.6990167238629700	2.7172248690424916	5.1154859399473445	T T T
-0.7094415448126001	4.1435052511823409	1.2500375407822586	F F F
-0.7059832491820599	1.2549183795437995	3.1700408560217461	T T T
1.8057052415015797	2.7490840239159651	5.1406450226288163	T T T
0.5435459591873999	1.9732672330073413	1.2500375407822586	F F F
-1.9593215545995297	3.4295836225092122	3.1641043933871260	T T T
3.0366903550986399	0.5601818372513311	5.1024824120025505	T T T
8.0614709831873981	1.9732672330073413	1.2500375407822586	F F F
5.5565986041909206	3.4085759007932714	3.1643870228545641	T T T
5.5661214345200705	0.5567094651032032	5.0988075504794441	T T T
6.8084834791873989	4.1435052511823409	1.2500375407822586	F F F

6.8156003329352703	1.2551789035964533	3.1550585825816806	T	T	T
4.2874226219260398	2.7395349419121868	5.1293373845630521	T	T	T
4.3025084711873998	4.1435052511823409	1.2500375407822586	F	F	F
4.2999524067509407	1.2545711935466042	3.1542104114933616	T	T	T
6.8146982270399388	2.7168776743643441	5.1075709296976557	T	T	T
5.5554959751873998	1.9732672330073413	1.2500375407822586	F	F	F
3.0464133677233800	3.4155205235561987	3.1658004811463596	T	T	T
8.0969056251709706	0.5290172279912901	5.1344259022581573	T	T	T
0.5435459591874001	6.3137432693573405	1.2500375407822586	F	F	F
-1.9933027711740605	7.7818660054256945	3.1355530786499868	T	T	T
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-3.2172207646032600	7.0547492514734929	5.1276414946840214	T	T	T
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-0.7105940727904798	7.1529306631585925	4.9925173300491759	T	T	T
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0.5449494154547803	4.9150682887658208	5.1505390045225798	T	T	T
5.5554959751873998	6.3137432693573405	1.2500375407822586	F	F	F
3.0435567115847100	7.7816052209444786	3.1530796109376049	T	T	T
3.0345351965439598	4.9620323783743618	4.9851676352715639	T	T	T
4.3025084711873989	8.4839812875323410	1.2500375407822586	F	F	F
4.3307757239310893	5.5696120316426416	3.1038924157420213	T	T	T

1.7987387211944403	7.0634300993747683	5.1143553372717898	T T T
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3.0495209671874002	6.3137432693573405	1.2500375407822586	F F F
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POSCAR for NCT

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-5.0119500160	8.6809520727	0.0000000000
0.0000000000	0.0000000000	28.2686004639

C N

31 1

Direct

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