Supplementary information

Zn-single Atom Catalysts Enable the Catalytic Transfer Hydrogenation of *α, β*-Unsaturated Aldehydes

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Experimental

Preparation of ZIF-8, Zn/NC-T, Zn/NC-900-acid and ZnO samples

Briefly, 1.190 g $Zn(NO_3)_2 \cdot 6H_2O$ was dissolved in methanol and stirred for 10 min, and then it was quickly added into another methanol containing 1.314 g of 2-methylimidazole (MeIM). The mixture was stirred for 4 h at room temperature. The as-obtained ZIF-8 precursors were centrifuged and washed with methanol three times. Finally, the sample was vacuum-dried at 60 °C overnight and kept for usage. The as-obtained ZIF-8 samples were placed in a porcelain boat. It was then sintered at certain calcination temperatures for 1 h under an N_2 atmosphere with a heating rate of 5°C /min. The calcination temperature was set at 700°C, 800°C, 900°C, and 1000°C, respectively. Thus, the corresponding collected samples were named Zn/NC-700, Zn/NC-800, Zn/NC-900, and Zn/NC-1000, respectively. In the case of the preparation of Zn/NC-900-acid catalyst, the Zn/NC-900 (100 mg) sample was immersed into the aqueous solution of HCl (0.5 mol/L, 10 mL). Then, they were stirred at 80 °C for 5 h. After that, the solid sample was washed using deionized water to remove the residual acid. The pH of the final solution was controlled to be about 7.0. The Zn species contained in the Zn/NC-900-acid catalyst was 2.6 wt.%, measured by ICP. In addition, as for the synthesis of the ZnO sample, the as-obtained ZIF-8 precursors were placed in a ceramic boat, and they were sintered in a muff furnace at 400 °C for 1 h under ambient atmosphere with a rate of 5 °C /min. After cooling to room temperature, the ceramic boat was transferred to a tube furnace, and then, they were sintered at 900°C for 1 h under a N_2 atmosphere with a rate of 5 °C /min. Finally, a powder of light-yellow color was obtained.

Evaluation of catalytic performance

Selective hydrogenation reactions

Selective hydrogenation reactions of cinnamaldehyde (CAL) were conducted in a 50 ml round bottom flask, which was loaded with 60 mg of catalyst, 49 mg of CAL, and 35 mL of isopropyl alcohol (IPA). A spherical condenser tube was connected to the flask. Prior to running the reaction, the system was evacuated with double-row tube equipment, and then filled with nitrogen, and the evacuated cycle was repeated at least three times. Finally, a nitrogen-filled balloon was equipped over the condenser tube to keep the N_2 atmosphere. After that, the reaction system was heated to the reaction temperature (80 °C) with a stirring speed of 600 rpm. Five hours later, the liquid mixture was separated from the solid catalyst by filtration method. The final products were analyzed using an Agilent 7890B gas chromatograph (GC) equipped with an FFAP capillary column, an auto-injector, and a flame ionization detector (FID). The mass fragmentation analysis of products for IPA-d8 and TBA was conducted on a gas chromatography-mass spectrometry (GC-MS, Agilent 7200 Q-TOF) with a DB-1701 capillary column. The conversion of CAL and selectivity of COL were obtained according to the following equations (1 and 2)[1]:

$$\text{Conversion of CAL (\%)} = \frac{\text{moles of CAL before reaction} - \text{moles of CAL after reaction}}{\text{moles of CAL before reaction}} \times 100\% \quad (1)$$

$$\text{Selectivity of COL (\%)} = \frac{\text{moles of Production}}{\text{moles of CAL consumed}} \times 100\% \quad (2)$$

In the case of the hot filtration experiment, the catalytic transfer hydrogenation reaction between CAL and IPA catalyzed by Zn/NC-900 catalyst was suspended after they were heated for 30 min. Then, the catalyst was removed from the reaction solution by the filtration method. The supernatant was allowed to be stirred for an additional 11.5 hours under the same reaction conditions. The conversion of CAL and selectivity

of COL at 0.5 h and 12 h were checked using a GC approach, respectively. Furthermore, as for the poisoning acid- and base-sites experiments, excess of KSCN and HCOOH was added into the reaction solution, respectively.

Isopropanol-D_1 [$CH_3CH(OD)CH_3$], and the mixture of isopropanol-D_8 [$CD_3CD(OD)CD_3$] and tert-butanol with a volume ratio of 1:3 were used as solvents for the CTH reactions to confirm the reaction mechanism[2-3]. It should be noted that in the mixed solvents, the tert-butanol can exchange H with D in the isopropanol-D_8 to yield $CD_3CD(OH)CD_3$[4]. The mass fragmentation analysis of final products was further conducted using a GC-MS (Agilent 7200 Q-TOF, with a DB-1701 capillary column)

Stability test of Zn-based SACs toward catalytic transfer hydrogenation

In the case of the stability test of Zn-N-C SACs, the reaction solution was filtered after each run, and the catalyst was washed using IPA to remove the organic molecules adsorbed on the surface of the catalysts. Finally, the catalysts were dried in a drying oven overnight. Prior to the next cycle of the catalysis test, the catalyst was heated at 400 °C for 1 h under a N_2 atmosphere with a heating rate of 5°C/min to remove the organic chemicals, which were strongly adsorbed at the active sites of the catalysts. A certain amount of CAL was added into the three-neck round flask according to the mass ratio between the Zn species of Zn-SAC and CAL used in the 1st run. The catalytic reaction was conducted under the same conditions as those for the 1st run.

CTH reactions of *α, β*-unsaturated aldehydes

The CTH reactions for various α, β-unsaturated aldehydes catalyzed by the Zn/NC-900 catalyst were also investigated. The reactions were conducted for a certain time at several temperatures, and those products were quantified by GC or ^{1}HNMR. Typically, hexanol, benzyl alcohol, and cyclohexanol were used as the hydrogen donor for the

transfer hydrogenation reaction of cinnamaldehyde. Those reactions were carried out at 140 °C for 11 hours. In addition, in the case of 3-methyl-2-butenal (31 mg) as the reactant, the mass of the catalyst was 100 mg, and the reaction was run at 80 °C for 11 h. Moreover, the reactions of 3-methyl-2-butena, furfural, α-methylcinnamaldehyde and various alcohols containing β-H as hydrogen sources were quantified using the GC method. The products for IPA and 4-nitrocinnamaldehyde, 4-methoxycinnamaldehyde, α-amylcinnamaldehyde and 5-hydroxymethylfurfural were quantified by ^{1}HNMR technique, with trimethoxybenzene as the internal standard substance.

Characterization

The morphologies and sizes of the as-prepared Zn/NC-T catalysts were characterized with a JEM-1200EX (JEOL) TEM operated at 100 kV. Electron energy loss spectra (EELS) of the samples were recorded by using a Tecnai G2 F20 UTWIN TEM equipped with a field emission gun. High-angle annular dark field (HAADF) scanning transmission electron microscopy (STEM) characterizations were performed with a spherical aberration-corrected instrument (FEI-Themis Z) operated at 200 kV. The Powder X-ray diffraction (XRD) patterns were recorded on a Bruker AXS D8 Advance X-ray diffractometer with Cu Kα radiation. The contents of Zn species contained in the Zn/NC-T catalysts were determined by an inductively coupled plasma atomic emission spectrometer (ICP-OES, Thermo Fisher ICAP-6300). Prior to the measurement, all samples were dissolved in the aqua regia for the nitration process, and the solutions were diluted to a certain concentration for testing. Characterization of the catalysts by the Brunauer-Emmett-Teller (BET) method was carried out on an ASAP 2460 instrument. The X-ray photoelectron spectroscopy (XPS) was carried out on a Thermo Scientific K-Alpha photoelectron spectrometer. The X-ray absorption spectra (XAS) of

the Zn K-edge were measured at the 1W1B station of the Beijing Synchrotron Radiation Facility (BSRF, 2.5 GeV, 250 mA, monochromatized with Si (111) double-crystals). Moreover, the N K-edge of the Zn/NC-900 sample was collected at the Beijing Synchrotron Radiation Facility (BSRF) line 4B9B station.

The FT-IR spectra of substrates chemically absorbed on the catalysts were collected on an integrated FOLI 20-Z Fourier transform infrared spectrometer equipped with a VeeMAX III specular reflection attachment. The catalysts were first mixed with anhydrous ethanol and naphthol solution to form a slurry, which was repeatedly coated on the glass carbon electrode in a small amount, and the electrode was dried under an infrared lamp. Then, the corresponding substrate or their mixtures were dropped onto the glass carbon electrode which was coated by different catalysts, respectively. Prior to the measurement, the electrodes coated with catalysts adsorbed by substrates were purged for a while using an inert gas with the aim of removing the physically adsorbed substrates on the catalysts surface. Finally, the signals were collected at a certain time interval under the atmosphere of inert gas for each catalyst and substrate. As for the reference signals, the different substrate or their mixtures on the glassy carbon electrode were also measured according to the same procedure. *In situ* FT-IR experiments were conducted on a Bruker TENSOR 27 equipped with an MCT narrow-band detector and a self-made temperature-controlled gas-liquid-solid reaction cell (Beijing Scistar Technology Co. Ltd.). The reactants in the system were diluent in an equal proportion using tetrachloroethylene. Prior to running the reaction, the deduction of background absorption was performed. The reaction temperature of system increased gradually via heating. When it reached the reaction temperature, the IR signals of reactants and products were collected at various reaction times.

DFT calculations

All first-principles calculations were performed using the Vienna Ab-initio Simulation Package (VASP)[5-6]. The exchange-correlation energy was approximated by the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) functional[7-8]. Spin polarization as well as vdW-dispersion energy-correction of DFT-D3 were considered[9-10]. A periodically projected plane wave basis set was employed using the projector-augmented wave (PAW) method with a kinetic energy cutoff of 500 eV, and with a Monkhorst-Pack *k*-point grid of 3 × 3 × 1 for the Brillouin zone sampling for structural optimization. The convergence criterion for the self-consistent iteration was 1×10^{-4} eV. The ionic relaxations can be terminated when the force on each atom is less than 0.02 eV/Å. The single-atom catalyst model is built based on a graphene structure containing Zn-N moiety with lattice dimensions of 17.04 × 19.68 Å in the basal plane and 15 Å in a perpendicular direction to ensure a sufficiently large vacuum. This system size is found to be sufficiently large to eliminate the interaction energies between the neighboring metals due to periodical structure. The formation energy of the model catalyst was calculated as:

$$E_f = E_{M\text{-}N\text{-}C} + xE_C - E_{gra} - \frac{y}{2}E_{N_2} - E_M \qquad (3)$$

Where E_f represents the formation energy. $E_{M\text{-}N\text{-}C}$ and E_{gra} represent the energy of the optimized M-N-C catalyst and graphene, respectively. E_C refers to the energy of a single carbon atom in graphene, and x represents the number of C atoms; E_{N_2} represents the energy of nitrogen, y represents the number of N atoms. E_M represents the energy of a single metal atom in metal bulk. The adsorption energy was calculated as

$$\Delta G = G_{total} - G_{gra} - G_{molule} \qquad (4)$$

Where G_{total} represents the total energy of the whole system when the reaction intermediates are adsorbed at the active site. G_{gra} represents the energy of the initial catalyst without adsorbing intermediates. G_{molule} represents the energy of the intermediate of the reaction.

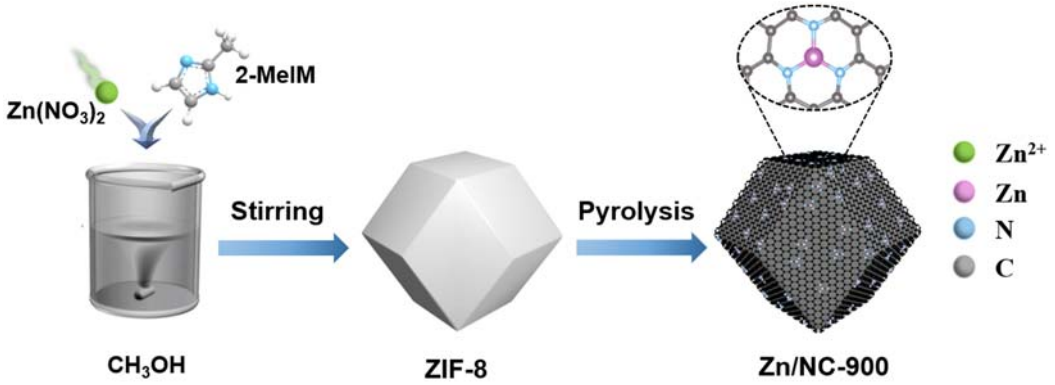


Figure S1. Schematic diagram for the synthesis of Zn-N-C single-atom catalysts (SACs).

Table S1. The contents of Zn, N, C and O species contained in various Zn-based catalysts measured by ICP-MS and XPS.

Catalysts	Zn / wt.% (ICP)	Zn / wt.% (XPS)	N / wt.% (XPS)	C / wt.% (XPS)	O / wt.% (XPS)
Zn/NC-700	24.3	20.0	15.1	53.8	11.1
Zn/NC-800	14.6	18.2	14.3	54.2	13.3
Zn/NC-900	12.0	10.9	11.3	68.3	9.5
Zn/NC-1000	5.7	6.2	7.0	76.8	10.0

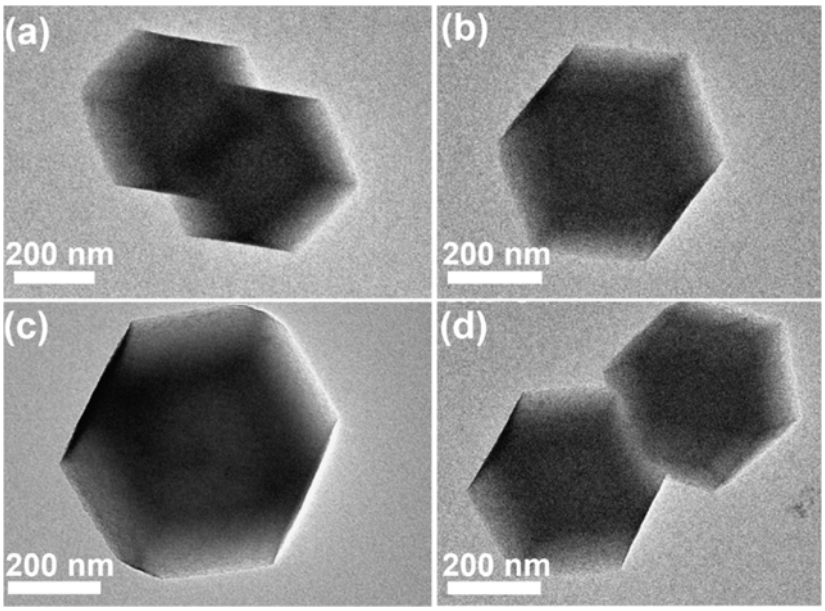


Figure S2. TEM images of Zn/NC catalysts prepared at different calcination temperatures: (a) Zn/NC-700; (b) Zn/NC-800; (c) Zn/NC-900 and (d) Zn/NC-1000.

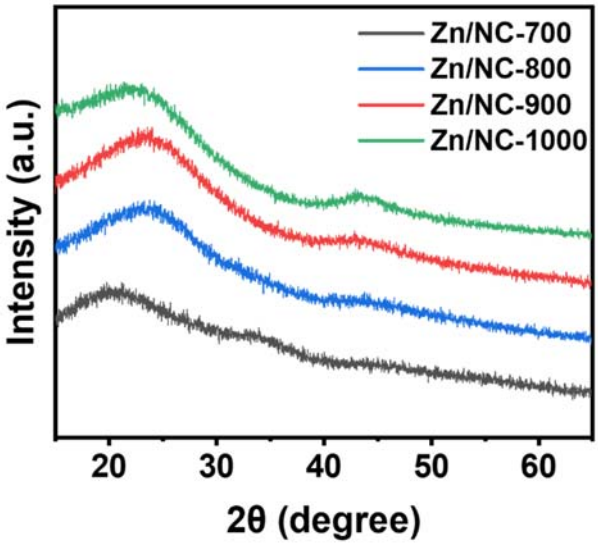


Figure S3. XRD patterns of Zn/NC catalysts prepared at different calcination temperatures.

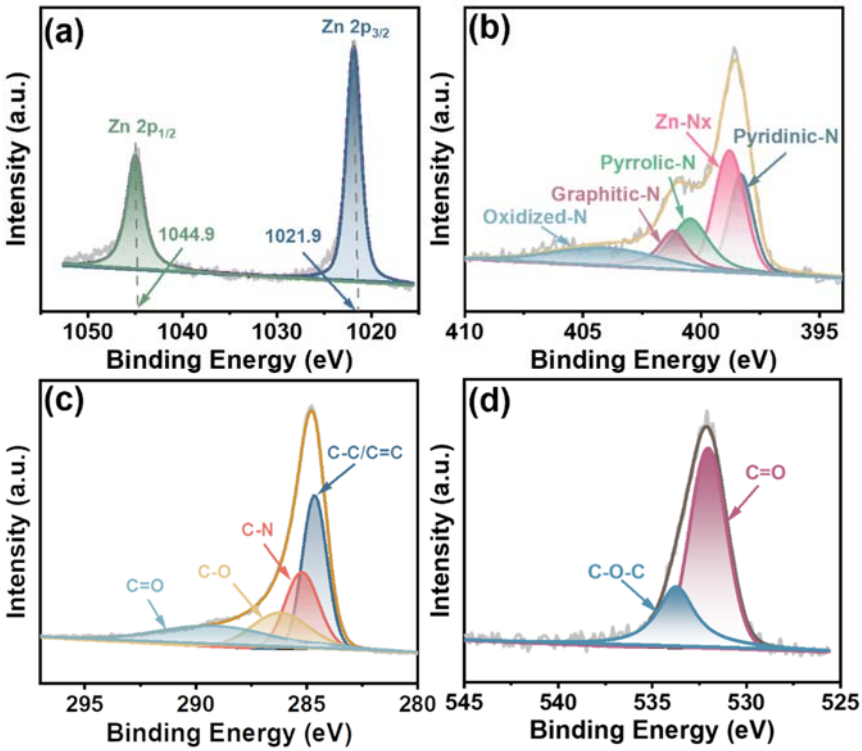


Figure S4. XPS spectra of Zn/NC-900 single atom catalyst: (a) Zn 2p; (b) N 1s; (c) C 1s; (d) O 1s.

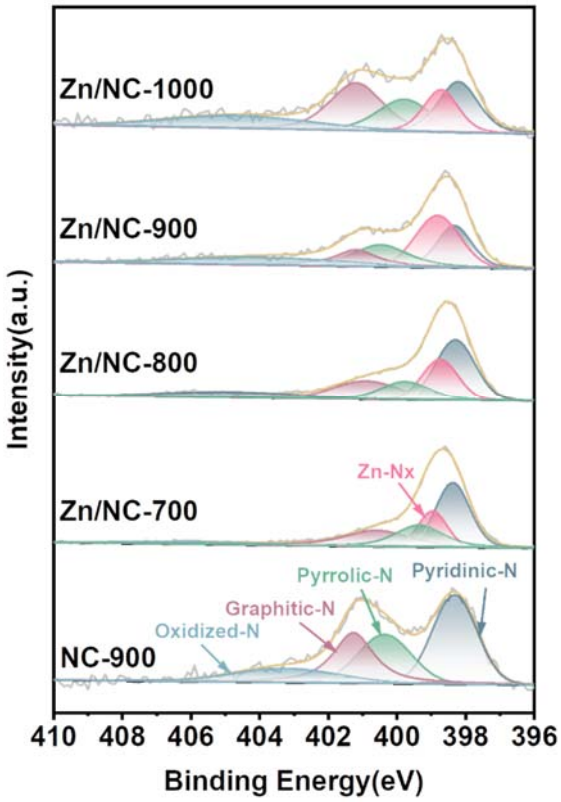


Figure S5. The XPS spectra for N 1s in the reference NC-900, and various Zn/NC samples prepared at different calcination temperatures.

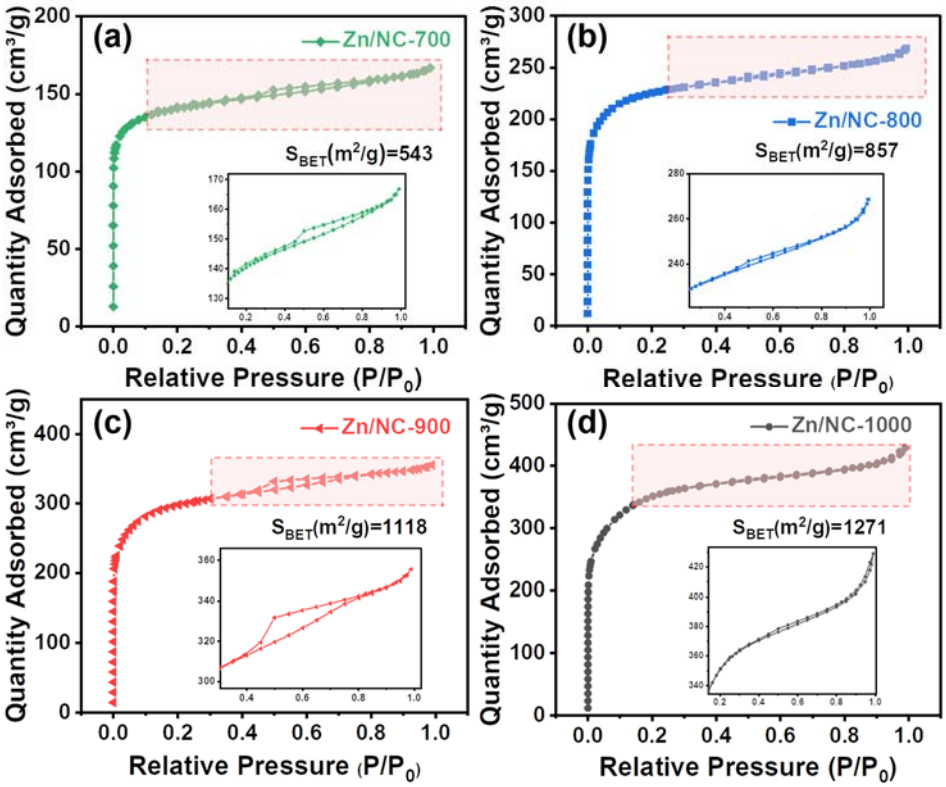


Figure S6. The N_2 adsorption–desorption isotherms of Zn/NC catalysts prepared at different calcination temperatures: (a) Zn/NC-700; (b) Zn/NC-800; (c) Zn/NC-900; and (d) Zn/NC-1000.

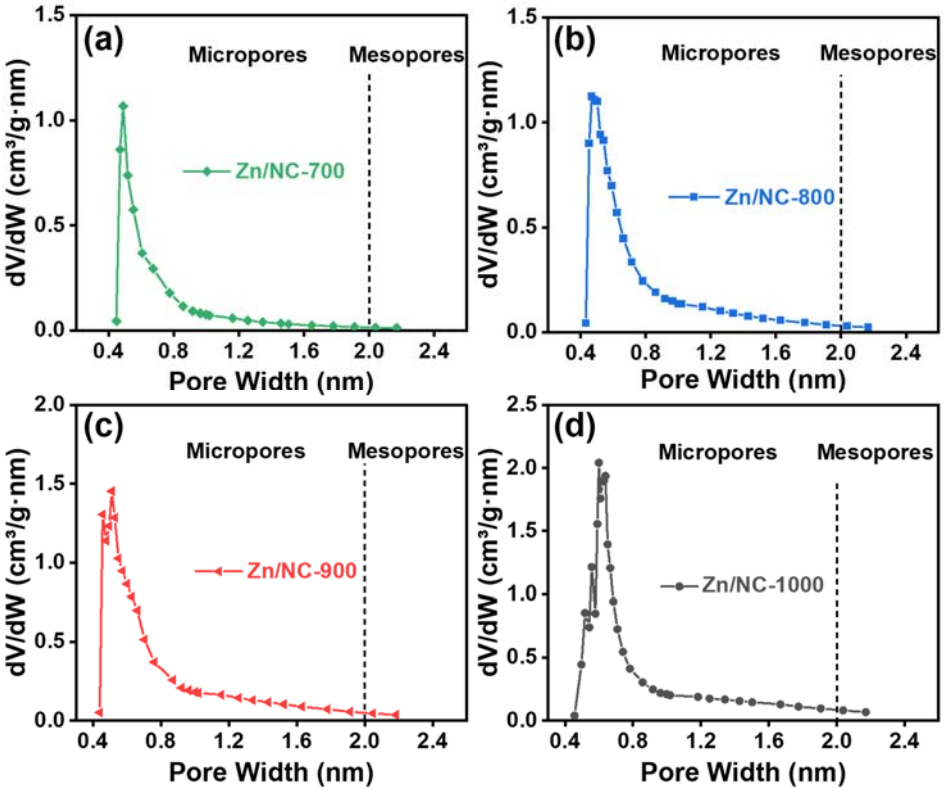


Figure S7. The pore size profile of Zn/NC catalysts prepared at different calcination temperatures: (a) Zn/NC-700; (b) Zn/NC-800; (c) Zn/NC-900; and (d) Zn/NC-1000.

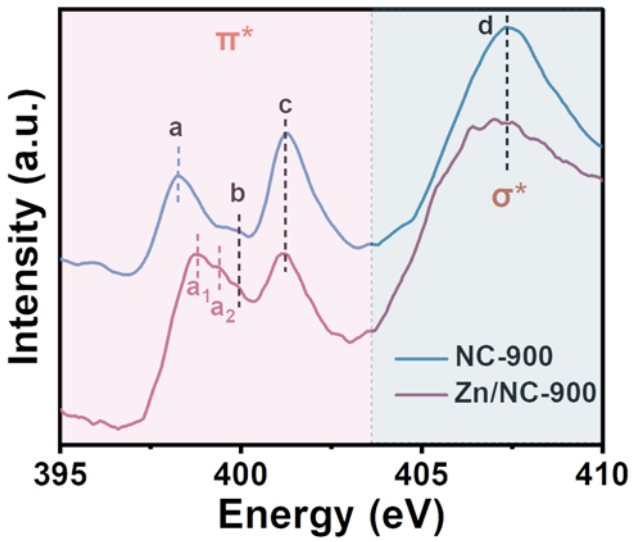


Figure S8. N K-edge XANES spectra of Zn/NC-900 catalyst and reference N-C sample.

Table S2. EXAFS fitting parameters at the Zn K-edge for Zn/NC samples (S_0^2= 0.84).

Sample	Path	C. N.[a]	R (Å)[b]	σ²×10³ (Å²)[c]	ΔE (eV)[d]	R factor
Zn foil	Zn-Zn	6*	2.65±0.01	9.8±0.7	1.1±1.3	0.002
	Zn-Zn	6*	2.78±0.03	20.4±2.7		
ZnO	Zn-O	3.7±0.6	1.97±0.01	4.1±1.6	4.4±2.0	0.014
	Zn-Zn	10.4±1.9	3.23±0.01	12.8±1.4	2.6±1.5	
ZnPc	Zn-N	4.1±0.5	1.99±0.01	3.2±0.9	10.7±1.7	0.012
	Zn-C	5.7±1.8	2.99±0.02	2.3±2.0	11.1±2.3	
Zn/NC-700	Zn-N/C1	3.2±0.3	1.86±0.01	5.7±0.6	1.0±0.2	0.007
	Zn-N/C2	3.9±0.5	1.96±0.01	6.5±0.8	1.0±0.2	
Zn/NC-800	Zn-N/C	4.1±0.6	1.96±0.01	4.1±0.5	1.0±0.2	0.006
Zn/NC-900	Zn-N/C	3.2±0.5	1.95±0.01	3.8±0.5	1.0±0.2	0.005
Zn/NC-1000	Zn-N/C	2.9±0.5	1.96±0.01	4.8±0.5	1.0±0.2	0.007
Zn/NC-900-used	Zn-N/C	3.1±0.5	1.96±0.01	5.1±0.5	1.0±0.2	0.006

S_0^2 is the amplitude reduction factor; [a]*C.N*: coordination numbers; [b]*R*: bond distance; [c]σ^2: Debye-Waller factors; [d]*ΔE*: edge-energy shift. *R* factor: goodness of fit. *: fitting with fixed parameter.

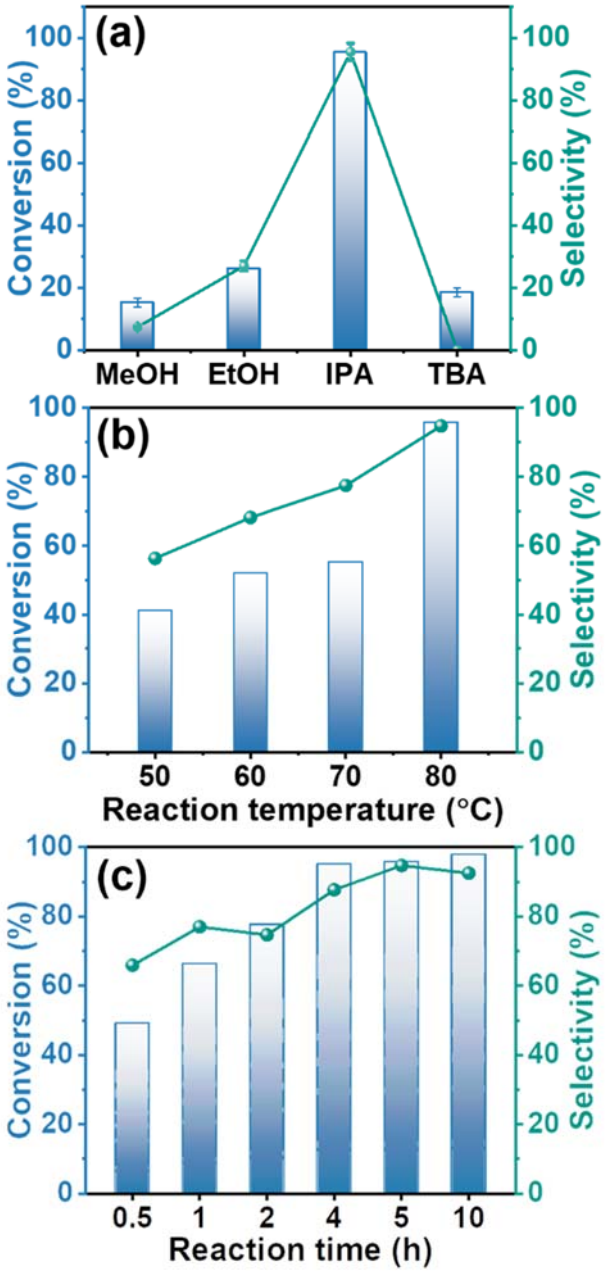


Figure S9. Optimization of the reaction conditions for the CTH reaction between CAL and alcohol: (a) solvent; (b) reaction time; and (c) reaction temperature.

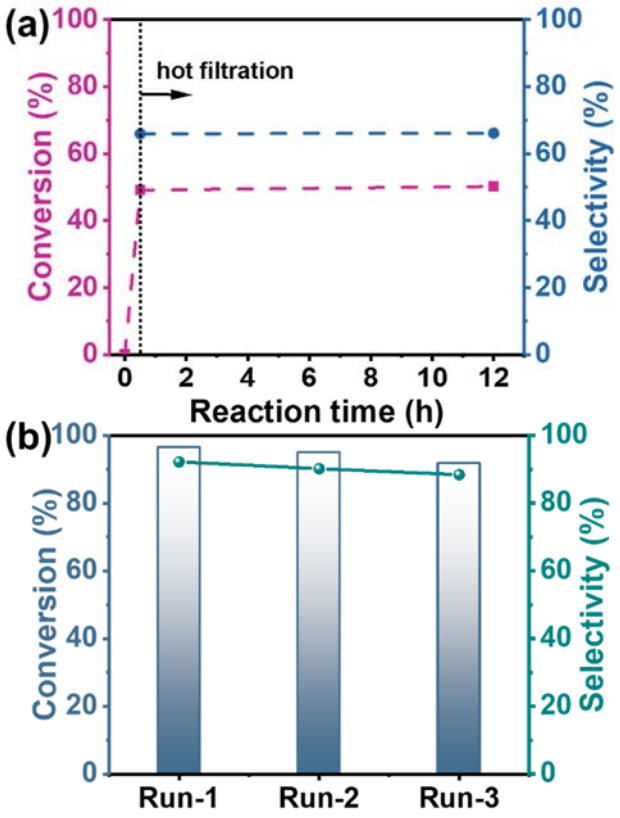
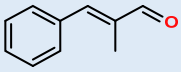
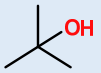
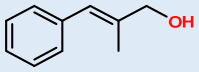
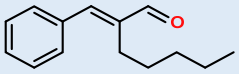
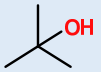
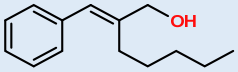
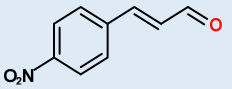
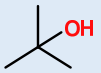
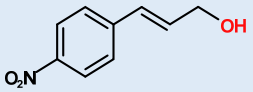
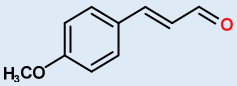
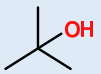
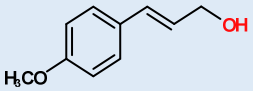
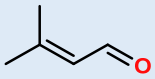
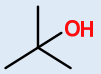
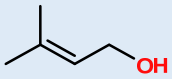
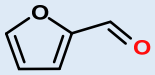
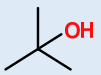
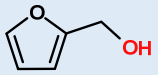
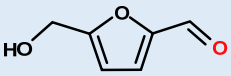
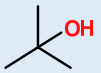
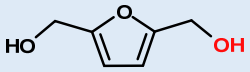
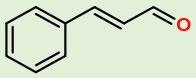
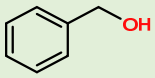
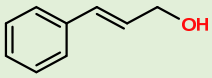
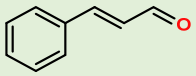
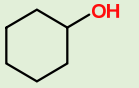
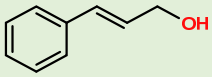
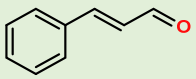
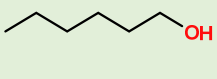
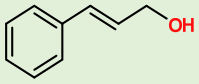


Figure S10. (a) Hot filtration test of CTH reaction between CAL and IPA; (b) stability evaluation of Zn/NC-900 catalyst towards selective transfer hydrogenation of CAL and IPA. Reaction conditions: 60 mg of Zn/NC-900 catalyst, 80 °C, 5 h, 49 mg of CAL.

Table S3. Catalytic transfer hydrogenation reactions of various *α, β*-unsaturated aldehydes with different alcohols over the Zn/NC-900 catalyst.

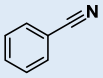
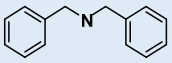
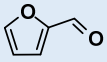
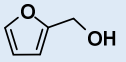
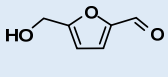
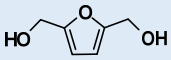
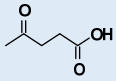
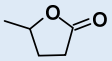
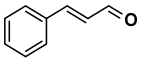
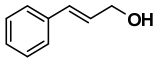
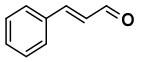
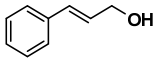
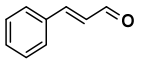
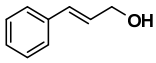
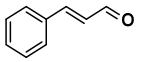
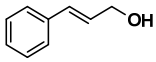
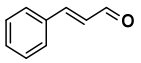
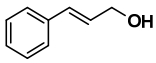
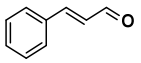
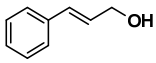
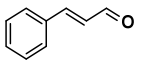
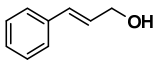
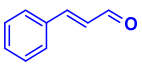
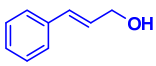
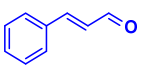
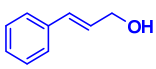
Entry No.	Substrate	Alcohol	Product	Conversion/ %	Selectivity/ %
1[a]				94.0	97.3
2[a]				93.3	98.1
3[a]				99.9	99.9
4[a]				89.6	83
5[b]				96.6	90.2
6[a]				99.4	88.7
7[a]				99.7	96.1
8[c]				93.3	93.7
9[c]				96.7	92.1
10[c]				90.3	81.7

[a] The molar ratio between reactant and Zn specie of catalyst was 6:1

[b] Reaction condition: 31 mg of substrate, 100 mg of catalyst (Zn/NC-900), 35 mL of IPA, 0.1MPa N_2, reaction temperature: 80 °C; reaction time: 11 hours

[c] Reaction condition: 48 mg of cinnamaldehyde, 60 mg of catalyst (Zn/NC-900), 5 mL of solvent, 0.1MPa N_2, reaction temperature: 140 °C, reaction time: 11 hours

Table S4. Various catalysts for CTH reaction of different *α, β*-unsaturated aldehydes with alcohols reported in the literatures.

Catalysts	Substrate	Product	Conv. /%	Sel. /%	Reaction condition	H donor	Reference
ISAS-Co/OPNC			99	99	toluene, 120 °C, 1.5h 0.1 MPa	HCOOH	*Angew. Chem. Int. Ed. 2018, 57, 11262*
Pd_1/ND@G			100	98	60 °C, 8h, MeOH sealed tube	NH_3BH_3	*Nat. Commun. 2021, 12, 6194*
Ru-CTF-I-900 (single atoms and clusters)			100	99	140 °C, 24h autoclave	IPA	*Adv. Sci., 2021, 8, 2001493*
Ni-SAs/NC			95.6	96.8	130 °C, 3h, 2MPa N_2	IPA	*J. Mater. Chem. A 2021, 9, 1110*
Zr_1/NC			~100	~100	130 °C, 2.5h autoclave	IPA	*Green Chem. 2022, 24, 6931*
Cu_1@UiO-66-$(COOH)_2$			100	96.7	140 °C, 1MPa N_2, 10h	IPA	*Chem. Eng. J.* 2023, *454, 140156*
CoO_x@Co NPs			97.5	90.1	120 °C, 8h, 0.1MPa N_2	IPA	*ChemCatChem 2020, 12, 1019*
Zr-BDB nanoparticles			96.9	97.2	100 °C, 6h stainless reactor	IPA	*Green Chem. 2021, 23, 1259*
Zr-tannin nanoparticles			95	97	80 °C, 4h pressure tube	IPA	*Green Chem. 2020, 22, 180*
Al_2O_3			97.8	96.8	120 °C, 12h, 1MPa N_2	EtOH	*ACS Sustain. Chem. Eng 2020, 8, 8195*
ZIF-67@SiO_2-CPTEOS			84.59	95.01	180 °C, 12h, 1MPa N_2	IPA	*J. Catal. 2020, 381, 468*
Pt NP/UiO-66			90.5	94.6	150 °C, 12h, 1MPa N_2	IPA	*ACS Appl. Nano Mater. 2020, 3, 12260*
Ni-SAs/ MgAlO-450			100	100	150 °C, 2h, 1MPa N_2	IPA	*J. Catal. 2021, 393, 1*
Zn/NC-900 ZnN_3 SAC			95.4	95.5	80 °C, 5h, 0.1MPa N_2	IPA	This work
Zn/NC-800 ZnN_4 SAC			85.9	84.4	80 °C, 5h, 0.1MPa N_2	IPA	This work

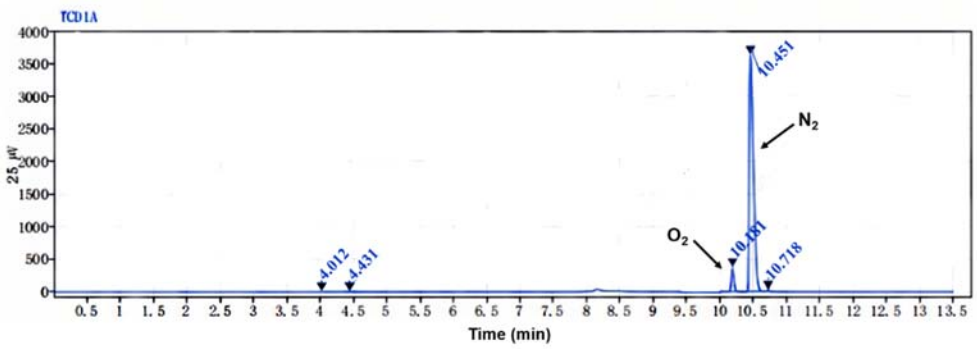


Figure S11. Chromatogram of final compositions for the isopropanol dehydrogenation experiment by GC with a TCD detector.

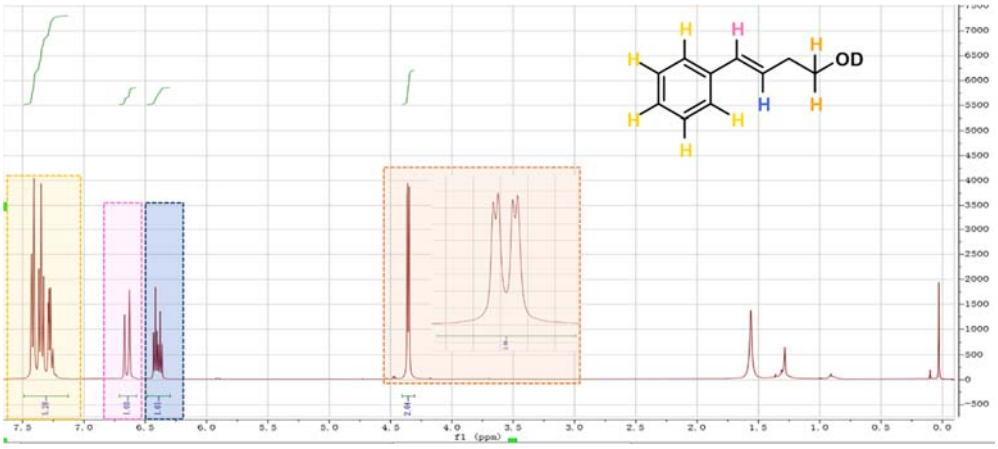


Figure S12. ^{1}HNMR of the products for the CTH reaction between CAL and IPA-d_1 ($CH_3CH(OD)CH_3$).

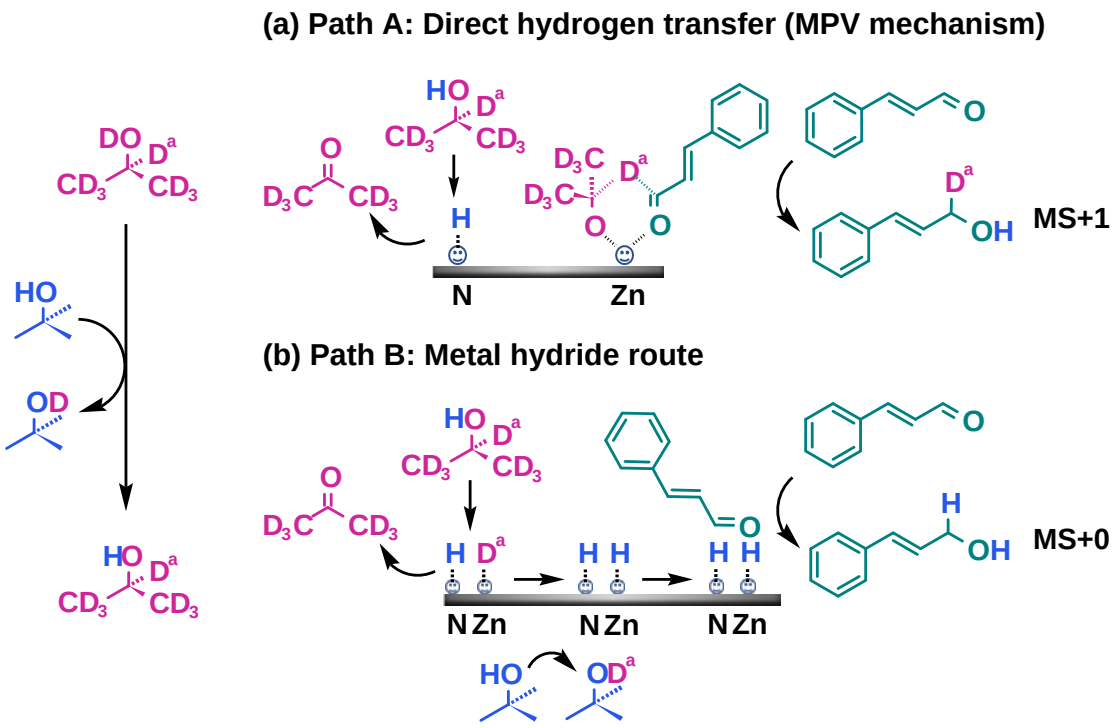


Figure S13. Scheme of the reaction mechanism for CTH reaction *via* direct hydrogen transfer route (Meerwein-Ponndorf-Verley, MPV mechanism, Path A) and metal hydride route (Path B).

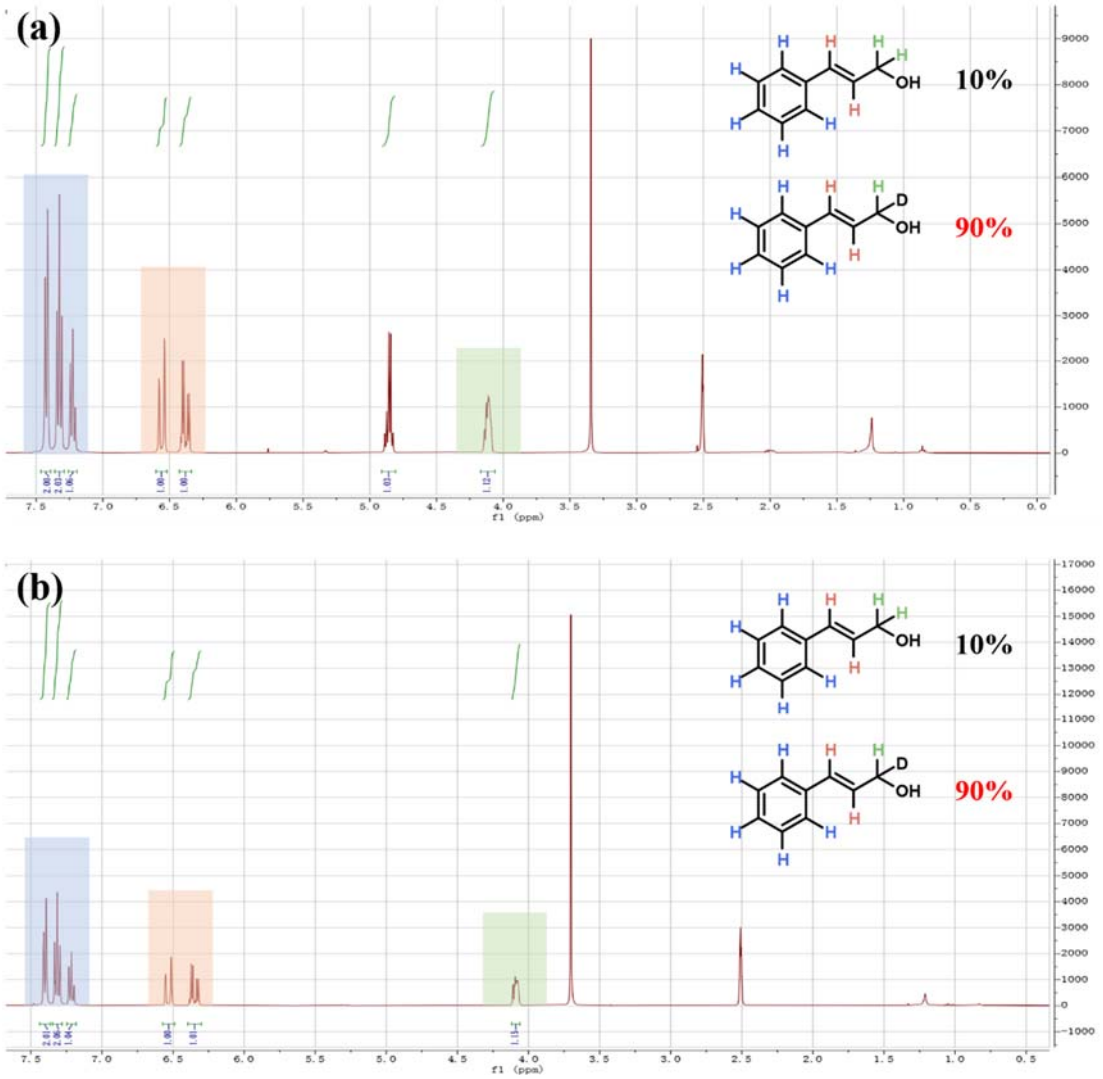


Figure S14. ^{1}HNMR for the deuteration experiments over catalysts Zn/NC-800 (a) and Zn/NC-900 (b), using the mixture of IPA-d_8 [$CD_3CD(OD)CD_3$] and TBA with volume ratio of 1:3 as solvent.

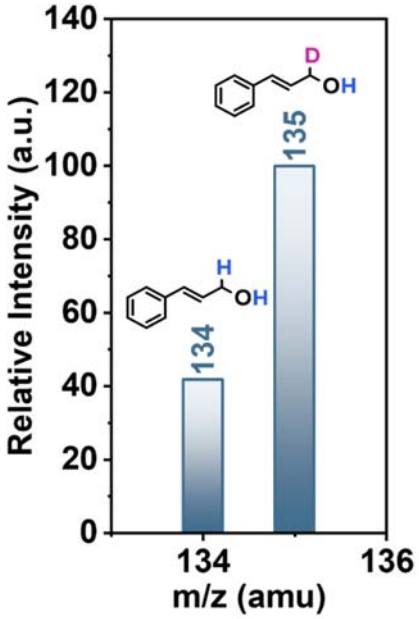


Figure S15. Mass fragmentation analysis of the products for the CTH reaction between CAL and mixed solvents of IPA-d_8 and TBA (volume ratio of 1:3) catalyzed by Zn/NC-900 SACs.

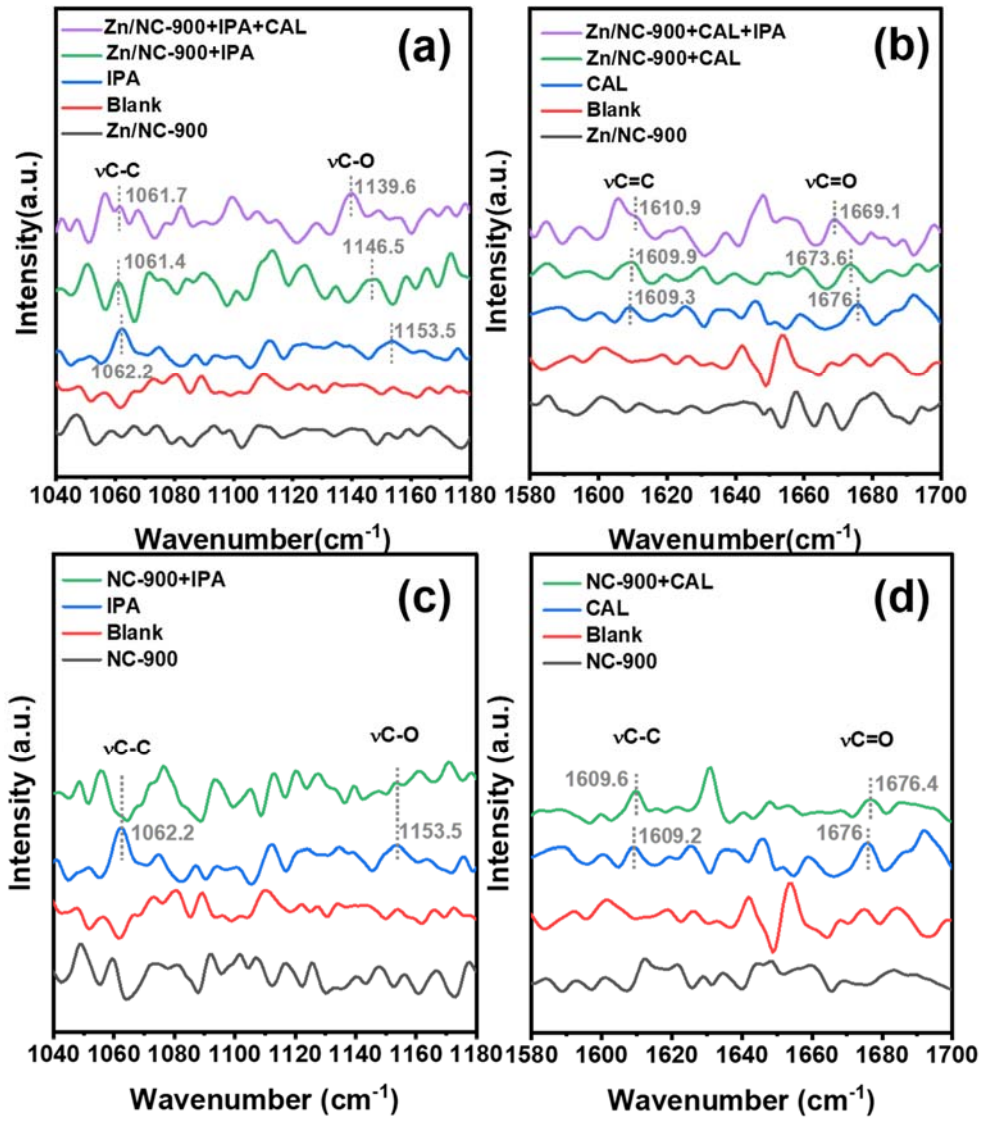


Figure S16. *FT-IR* spectra of isopropanol and cinnamaldehyde chemisorbed on the Zn/NC-900 SAC (a, b), and NC-900 (c, d) catalysts, respectively.

Table S5. The formation energy for ZnN_4 coordination configuration with different numbers of pyridinic-N and pyrrolic-N species.

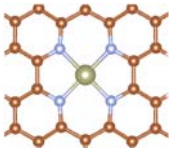
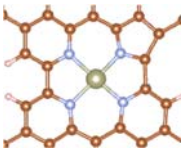
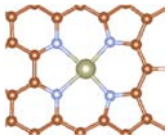
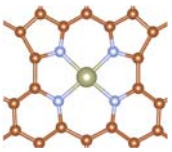
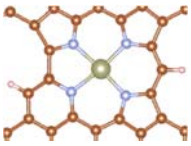
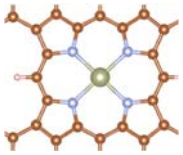
No.	Coordination	Structure	Formation energy/eV
1	Zn-4$N_{pyridine}$		-6.185
2	Zn-3$N_{pyridine}$-1$N_{pyrrole}$		-3.80
3	Zn-2$N_{pyridine}$-2$N_{pyrrole}$-1		-5.92
4	Zn-2$N_{pyridine}$-2$N_{pyrrole}$-2		-1.30
5	Zn-1$N_{pyridine}$-3$N_{pyrrole}$		-2.99
6	Zn-4$N_{pyrrole}$		-4.197

Table S6. The formation energy for ZnN_3 coordination configuration with different numbers of pyridinic-N and pyrrolic-N species.

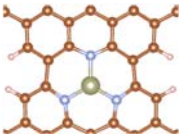
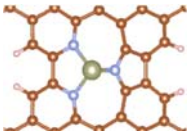
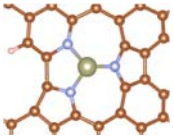
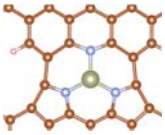
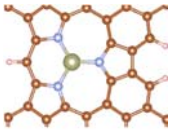
No.	Coordination	Structure	Formation energy/eV
1	Zn-3$N_{pyridine}$		-1.75
2	Zn-2$N_{pyridine}$-1$N_{pyrrole}$		-0.39
3	Zn-1$N_{pyridine}$-2$N_{pyrrole}$-1		1.73
4	Zn-1$N_{pyridine}$-2$N_{pyrrole}$-2		3.93
5	Zn-3$N_{pyrrole}$		-0.13

Table S7. The formation energy and adsorption configuration of isopropanol and cinnamaldehyde over the ZnN_4 SACs.

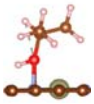
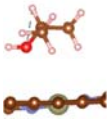
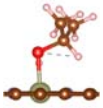
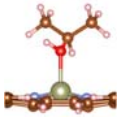
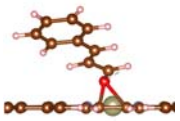
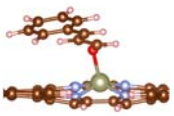
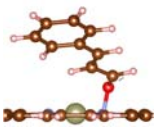
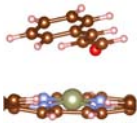
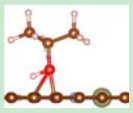
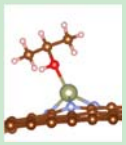
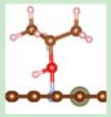
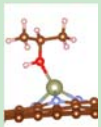
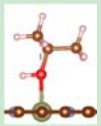
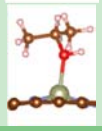
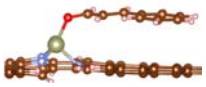
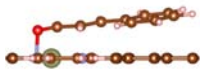
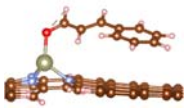
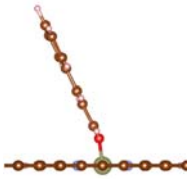
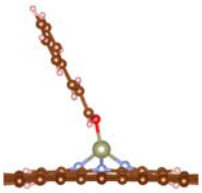
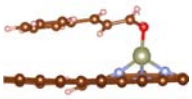
No.	Substrate	Adsorption site	Structure		Adsorption energy/eV
			Initial state	Final state	
1	Isopropanol	C			-0.067
		N			/
		Zn			-0.087
		Zn			-0.063
2	Cinnamaldehyde	C			-0.215
		N			/
		Zn			-0.37
		Zn			-0.078

Table S8. The formation energy and adsorption configuration of isopropanol and cinnamaldehyde over the ZnN_3-SACs.

No.	Substrate	Adsorption site	Structures		Adsorption energy/eV
			Initial state	Final state	
1	Isopropanol	C			-1.433
		N			-1.436
		Zn			-2.033
2	Cinnamaldehyde	C			-2.038
		N			-
		Zn			-1.913
		Zn			-2.053

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