# Supporting information

# IS Trace-Level Aluminum in Zeolite Matrix Catalytically Inert? A Case Study of Alcohol Dehydration in Dealuminated Beta Zeolite

Haoxi Jiang[a,b,c], Jiahao Guan[a,b,c], Changdong Li[a,b,c], Lingtao Wang[a,b,c], Guochao Yang[a,b,c,*]

a Key Laboratory for Green Chemical Technology of Ministry of Education, R&D Center for Petrochemical Technology, Tianjin University, Tianjin 300072, China

b Zhejiang Institute of Tianjin University, Ningbo, Zhejiang, 315201, China

c State Key Laboratory of Engines, Tianjin University, Tianjin 300072, China

E-mail: yang_gc@tju.edu.cn Phone: +86-22-27406119

1. Sample preparation

The dealuminated Beta zeolites were prepared by treating H-Al-Beta zeolite (Si/Al = 12, SINOPEC) with concentrated nitric acid (65-68%). Dealuminated Beta zeolite samples with varying aluminum contents were obtained by treating with concentrated nitric acid of different concentrations. In a typical acid treatment, 10.0g H-Al-Beta was stirred in 100 mL of 13M nitric acid at 363 K for 12 h. The recovered solids were washed with deionized water until neutral pH was achieved and subsequently dried overnight at 393 K.

B-Beta was prepared by hydrothermal method.[1] The synthesis was carried out with a gel composition of 1 $SiO_2$: 0.033 $B_2O_3$: 0.54TEAOH: 18 $H_2O$. The materials used were fumed silica, boric acid, TEAOH (25% aqueous solution). The gel was charged in Telfon-lined stainless steel autoclaves and heated at 423 K for 96 h. The collected precipitate was recovered by centrifugation, washed, dried at 393 K for 12 h and calcined at 823 K for 6 h to remove organic template.

DeB-B-Beta was obtained by treating B-Beta with 13mol· $L^{-1}$ concentrated nitric acid. The procedure is the same as the dealumination of H-Al-Beta.

Pure-silica zeolite F-Si-Beta was synthesized via a hydrothermal method modified from the procedure reported by Javier et al[2]. Specifically, 20.0 g of tetraethyl orthosilicate (TEOS) was added dropwise to 28.2 g of a 25% aqueous tetraethylammonium hydroxide (TEAOH) solution. The ethanol generated during hydrolysis, along with a portion of water, was evaporated. Subsequently, HF (40 wt%) was added to the mixture under manual stirring. The final gel exhibited a molar composition of $SiO_2$: TEAOH: HF: $H_2O$ = 1:0.5:0.5:7.5. The gel was transferred into

Teflon-lined stainless steel autoclaves and heated at 413 K for 120 h. The resulting precipitate was collected by centrifugation, washed thoroughly, dried at 393 K for 12 h, and calcined at 823 K for 6 h to remove the organic template.

2. Sample characterization

XRD patterns were recorded on a Rigaku Miniflex 600 diffractometer with Cu Kα radiation (λ = 1.54056 nm) at 40 kV and 15 mA. $N_2$ adsorption–desorption isotherms were measured at 77 K using a micromeritics Tristar 3000 instrument after degassing at 573 K for 6 h under vacuum. The Al content and Si content were determined by ICP-OES using an AgilentVarian-710ES. Prior to the analysis, samples were digested in an HF/HCl solution.

Magic angle spinning (MAS) nuclear magnetic resonance (NMR) spectra of $^{27}Al$ were collected on a Bruker Avance III 600 MHz Wide Bore spectrometer operating at a magnetic field of 14.2 T. The chemical shifts for $^{27}Al$ MAS NMR spectra were referenced to the aqueous solution of Al $(NO_3)_3$ (0 ppm). The $^{27}Al$ MAS NMR spectra were acquired at a spinning rate of 13 kHz with a π/12 pulse width of 1.2 μs and a recycle delay of 1 s, and the number of scans used was 10000.

Temperature-programmed desorption of $NH_3$ ($NH_3$-TPD) and isopropylamine (IPA-TPD) were performed on a Micromeritics AutoChem II 2920 chemisorption analyzer. For $NH_3$-TPD, approximately 100 mg of zeolite sample was first pretreated at 500 °C for 2 h in a helium stream (50 mL·$min^{-1}$) and then cooled to 100 °C. Saturated adsorption of $NH_3$ on the zeolite sample was achieved by introducing gaseous $NH_3$ (1 vol % in argon, 30 mL· $min^{-1}$) into the sample tube for 60 min. After that, the physically adsorbed $NH_3$ was removed by flushing the sample tube with the helium flow (50 mL· $min^{-1}$) at 100 °C for 4 h. To get the $NH_3$-TPD profiles, the zeolite sample was then heated up from 100 to 550°C at a ramp of 10 °C· $min^{-1}$; the amount of $NH_3$ released during heating for desorption was measured by a thermal conductivity detector (TCD)

and mass detector (Omistar, Pfeiffer). For isopropylamine-TPD, aproximately 20 mg of zeolite sample was pretreated at 500 °C for 2 h in a helium stream (50 mL· $min^{-1}$) and then cooled to 70 °C. Saturated adsorption of isopropylamine on the zeolite sample was achieved by pulsing isopropylamine 50 times. After that, the physically adsorbed isopropylamine was removed by flushing the sample tube with the helium flow (50 mL· $min^{-1}$) at 100 °C for 4 h. To get the IPA-TPD profiles, the zeolite sample was then heated up from 70 to 550°C at a ramp of 10 °C· $min^{-1}$. The profile of isopropylamine and propylene during heating was collected by mass detector (Omistar, Pfeiffer) with m/z=43 and 41 respectively

The OH-IR spectra were obtained on a Bruker Tensor 27 spectrometer equipped with a Hg-Cd-Te detector (MCT, 77 K) and high temperature chamber (Harrick), and 32 scans at 2 $cm^{-1}$ resolution were averaged in the 4000–400 $cm^{-1}$. The self-supporting wafer (~20 mg) was cleaned under vacuum at 673 K for 1 h and then cooled to 423K for 15min to collect the spectra. Backgrounds were subtracted with IR spectra collected with an empty IR cell under flowing He.

In situ DRIFTS experiment was conducted to gain insight into the catalytic mechanism of ethanol dehydration. In the typical procedure, dealuminated Beta zeolite was performed in an in-situ DRIFT cell using a zinc selenide (ZnSe) window and MCT detector. Prior to the experiment, the catalyst was activated by heat treatment at 500 °C for 2 h under 50 mL/ min of $N_2$. Then the catalyst was cooled down to 400 °C, and collect the background after stabilization for 1 h. The feed mixture consisted of ethanol vapor in $N_2$ flowing through the in situ DRIFT cell at a flow rate of 20 mL/ min . The

spectra were recorded for 32 scans with a resolution of 4 $cm^{-1}$

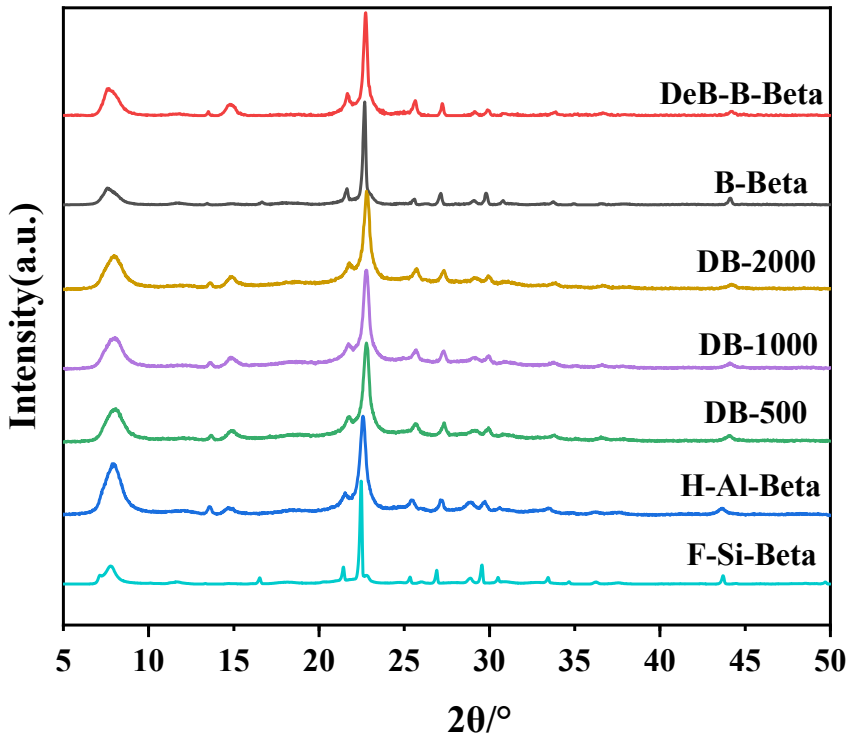



Figure S1 XRD profiles of different Beta zeolites

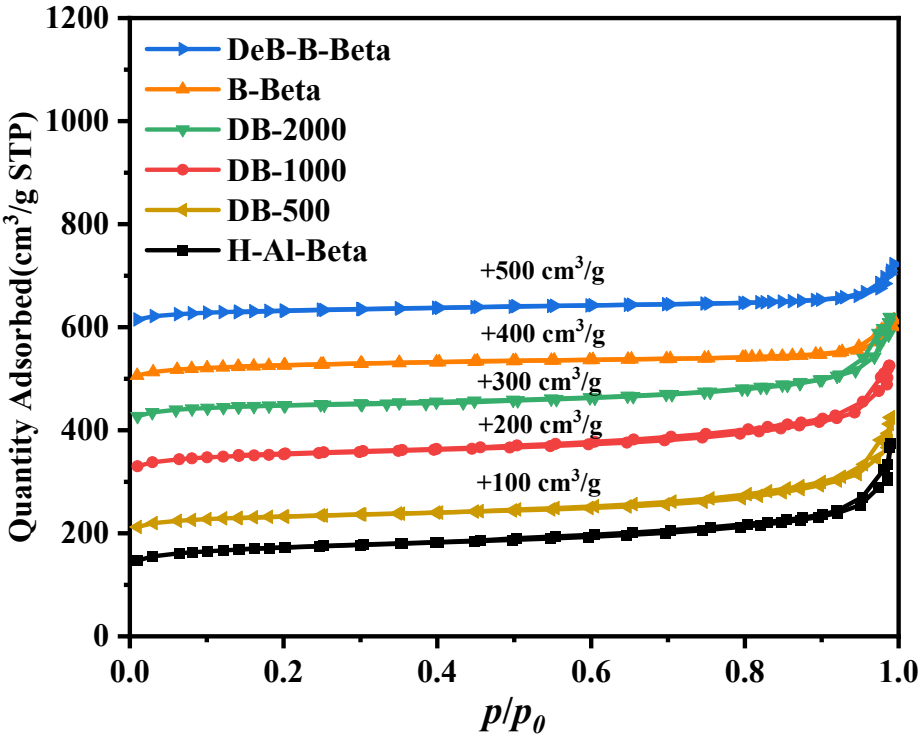



Figure S2 $N_2$ adsorption-desorption isotherms for different Beta samples

Table S1 Properties of different Beta zeolite samples

| Sample | Nitric acid concentration/M | Al(B) content/% | Si/Al(B) ratio | BET surface area/($m^{2/}$g) | Total pore volume/($cm^3$·/g) |
|---|---|---|---|---|---|
| H-Al-Beta | - | 3.367 | 12 | 532 | 0.447 |
| DB-500 | 6 | 0.079 | 460 | 410 | 0.378 |
| DB-1000 | 10 | 0.028 | 1025 | 475 | 0.427 |
| DB-2000 | 13 | 0.012 | 2123 | 487 | 0.432 |
| B-Beta | - | 1.097 | 12 | 389 | 0.265 |
| DeB-B-Beta | 13 | 0.026 | 578 | 405 | 0.271 |

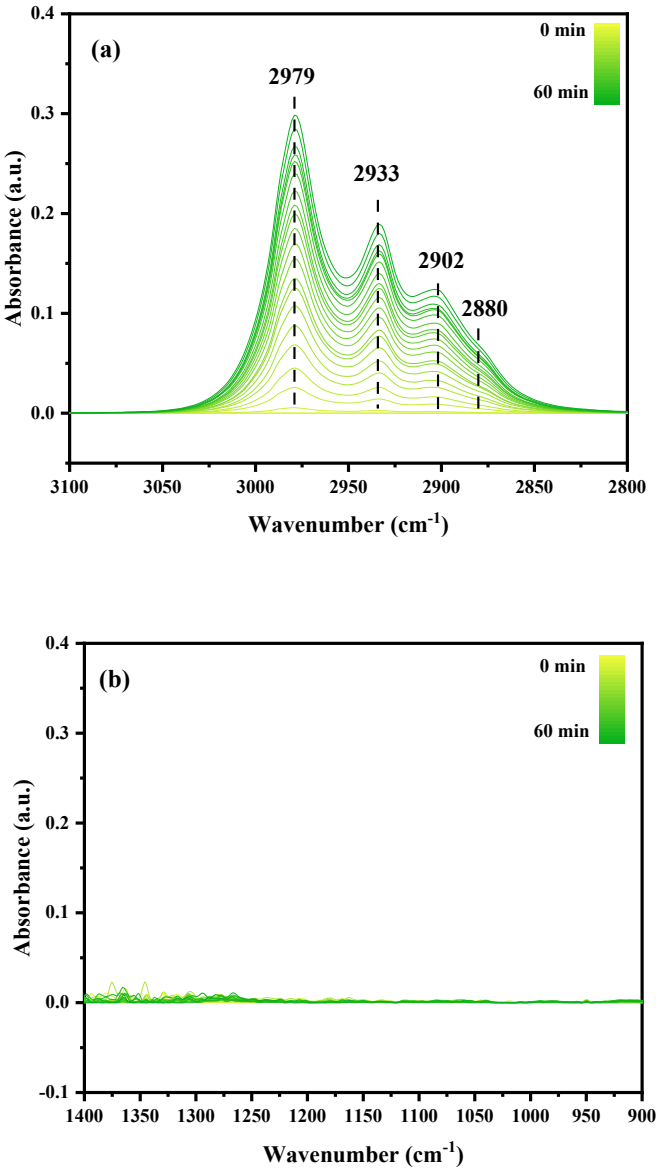



Figure S3 In situ DRIFTS spectra of C-H (a) and C-O (b)stretching vibration region of ethanol dehydration over DB-500

The C-H stretching vibration region of the in situ DRIFTS spectra (Figure S3a) revealed four distinct bands:2979 $cm^{-1}$ ($CH_3$ asymmetric stretching), 2979 $cm^{-1}$ ($CH_2$ asymmetric stretching), 2902 $cm^{-1}$ ($CH_3$ symmetric stretching), 2880 $cm^{-1}$ ($CH_2$

symmetric stretching)[3, 4] . The intensities of these peaks increased with reaction time, indicating the gradual accumulation of surface species containing $CH_2$ and $CH_3$. Within the ethanol dehydration system, such species could correspond to ethanol or reaction intermediates ethoxy species. Notably, in the C-O stretching vibration region (Figure S3b), no band associated with ethanol (1180 and 1060 $cm^{-1}$) were observed. This strongly suggests that the observed C-H vibrations originate from ethoxy species rather than adsorbed ethanol molecules. Since ethoxy intermediates only form via the Brønsted acid-catalyzed E1 mechanism (where dehydroxylation and dehydrogenation occur sequentially), while the E2 mechanism eliminates these steps synchronously without generating ethoxy species, our DRIFTS results support the dominance of the E1 pathway in this reaction.

3. Catalytic test

The dehydration performance of ethanol and n-butanol dehydration was carried out on a fixed-bed reactor. First, 0.5 g of loaded catalyst was activated at 673 K for 1 h with 100 mL· $min^{-1}$ $N_2$ flow. The alcohol feed was carried by 100 mL· $min^{-1}$ $N_2$ over the catalyst at 673 K and atmospheric pressure. The products were analyzed by a Shimadzu GC-2010 PLUS gas chromatograph equipped with an FID detector with an HP-Plot/Q column (30 m × 0.32 mm × 20 μm) with He as the carrier gas.

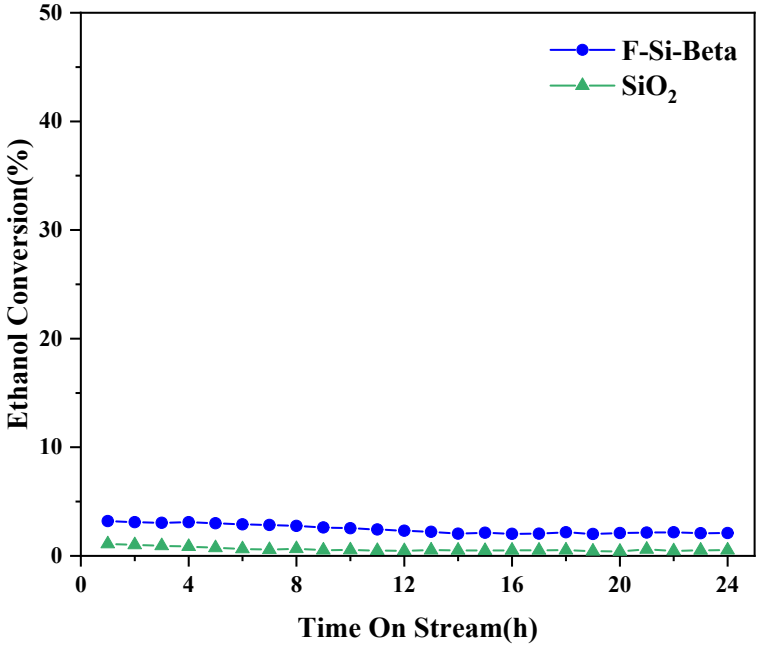



Figure S4 ethanol conversion of dehydration activity test for F-Si-Beta and $SiO_2$ (reaction condition: 400 °C, WHSV=4.5 $g_{ETOH} \cdot g_{cat}^{-1} \cdot hr^{-1}$))

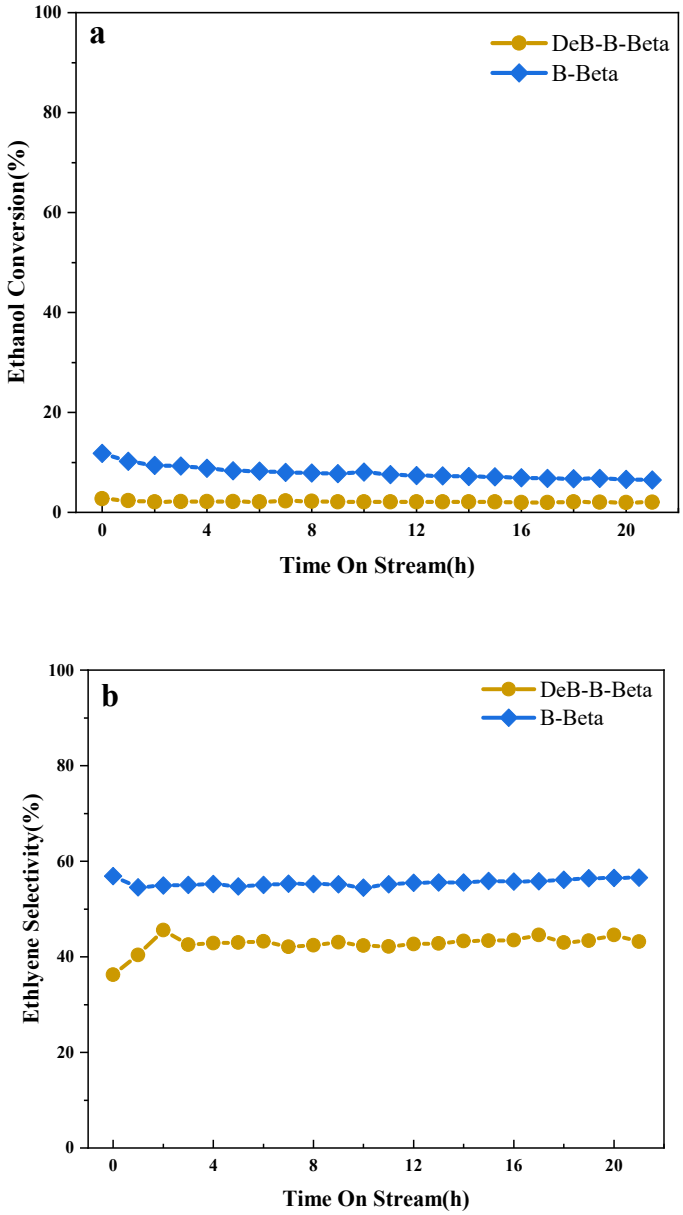



Figure S5 ethanol dehydration activity test for B-Beta and DeB-B-Beta: a: conversion, b: ethylene selectivity (reaction condition: 400 °C, WHSV=4.5 $g_{ETOH} \cdot g_{cat}^{-1} \cdot hr^{-1}$))

## 4. Computational Studies

### 4.1 Computational method

The dispersion correction periodic DFT is calculated by using Vienna ab initio software package (VASP) based on the plane wave basis set.[5, 6] The electronion interaction is described by the projector augmented wave method (PAW), and a plane-wave basis set with a cutoff kinetic energy of 520 eV was employed.[7, 8] The Brillouin zone sampling was restricted to the Γ-point in all the calculations. In all calculations, the generalized gradient approximation exchange correlation (XC) functional developed by Perdew, Burke, and Ernzerhof is used. The tolerance of the self-consistent field is $10^{-6}$ eV, and the maximum force convergence criterion is 0.03 eV/Å. The dispersion correction of the van der Waals interaction, the DFT-D3 method with Becke-Johnson damping function is adopted periodic calculations[9].

The transition states (TSs) were obtained by the "climbing-image" nudged elastic band and Dimer methods.[10, 11] The validity of each TS was confirmed by a single imaginary frequency of the normal modes at the saddle point. After the correction to zero-point energy (ZPE), the relative energy was calculated for each elementary step.[12]

### 4.2 Catalyst Model

This study used the BEA zeolite obtained from the International Zeolite Association (IZA) as the initial structure for theoretical calculations. The unit cell belongs to the tetragonal system $P4_122$. The unit cell parameters are a = b = 12.641 Å, c = 26.508 Å, α = β = γ = 90°, which contains 64 Si and 128 O atoms.

Previous experimental research have shown that in high silica-to-alumina ratio (Si/Al=75) zeolites, aluminum atoms predominantly occupy T1 and T2 sites.[13] Density

functional theory (DFT) calculations have also confirmed the difficulty of removing aluminum atoms from these two sites in beta zeolites, compared with other sites.[14]

Therefore, we selected T1 and T2 sites as the preferred locations for residual aluminum atoms in dealuminated beta zeolites. Further calculations were conducted to assess the adsorption energies of $NH_3$ and ethanol on Al-O(H)-Si sites modeled at T1 and T2 sites. As is shown in Table S2, the results did not show significant differences between the two models. To streamline unnecessary computational efforts, we chose the T2 site model (Figure S4) as the representation for residual Al-O(H)-Si sites in dealuminated beta zeolites.

To better compare the impact of site structure on activity, T2 was also selected as the dealumination site. As is shown in Figure S5 Si atom is removed to create silanol nest sites by saturating dangling oxygen atoms bonded to adjacent silicon atoms with hydrogen atoms.

Table S2 adsorption energy of $NH_3$ and ethanol on T1 and T2 Al-O(H)-Si sites

| Location | Molecular | $E_{ads}$/eV |
|---|---|---|
| T1 | $NH_3$ | -1.49 |
| | $C_2H_5OH$ | -1.26 |
| T2 | $NH_3$ | -1.48 |
| | $C_2H_5OH$ | -1.23 |

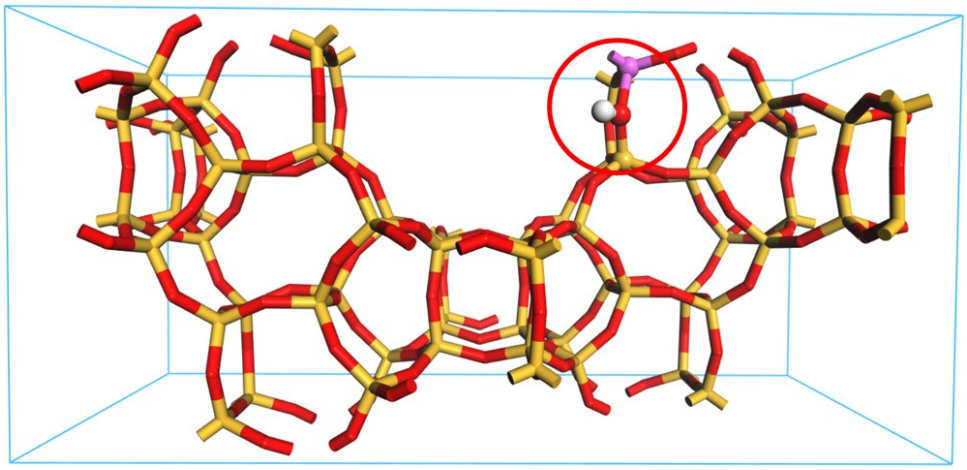


Figure S6 configuration of T2 Al-O(H)-Si site (Al, O, Si, H are depicted as purple, red, yellow and white)

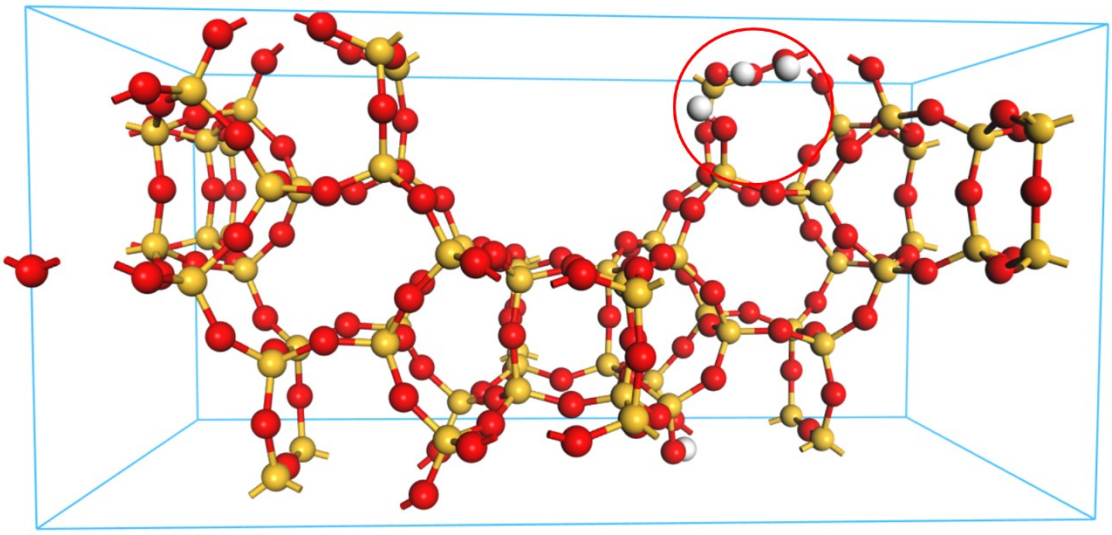
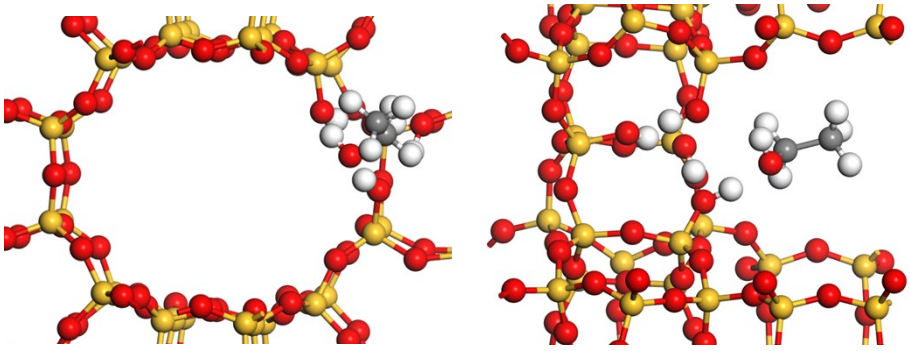
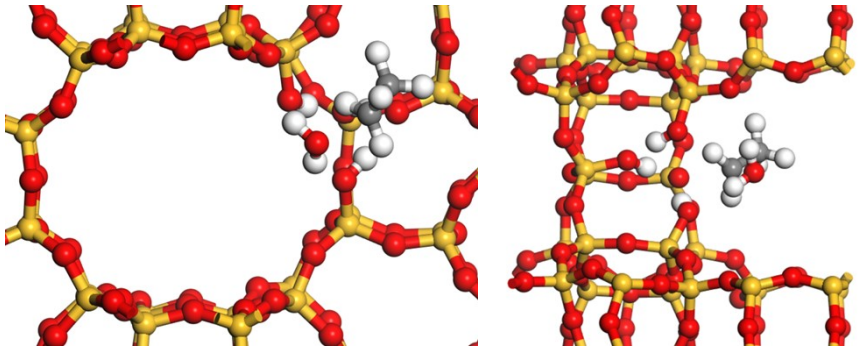


Figure S7 configuration of T2 silanol nest site (O, Si, H are depicted as red, yellow and white)

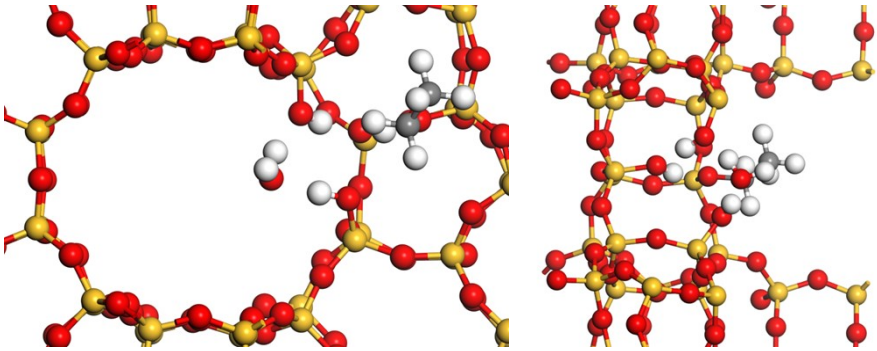
4.3 Configuration of ethanol dehydration on T2 silanol nest site (left: top view, right: side view)



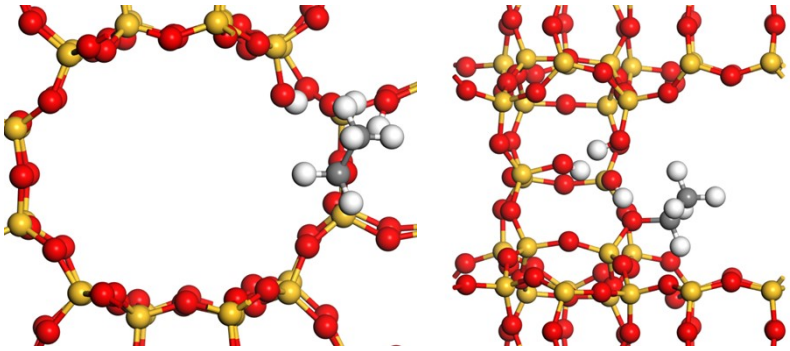
**S2**



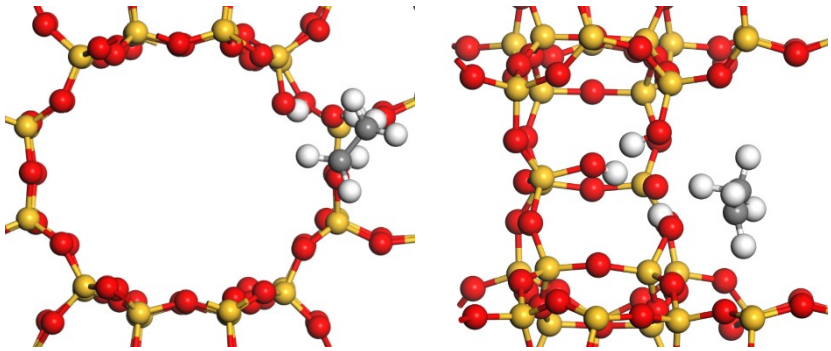
**TS1**



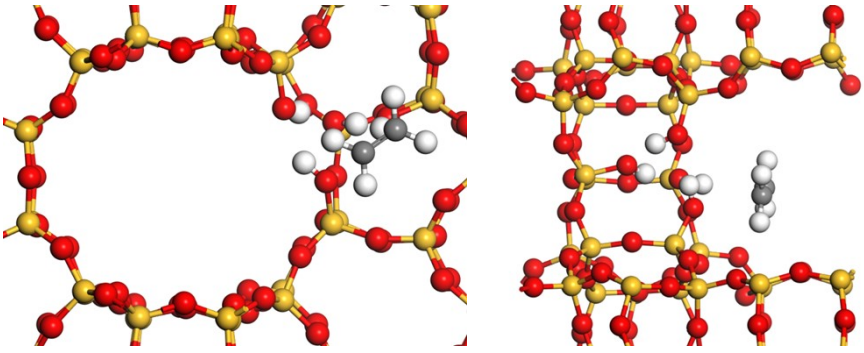
**S3**



**S4**

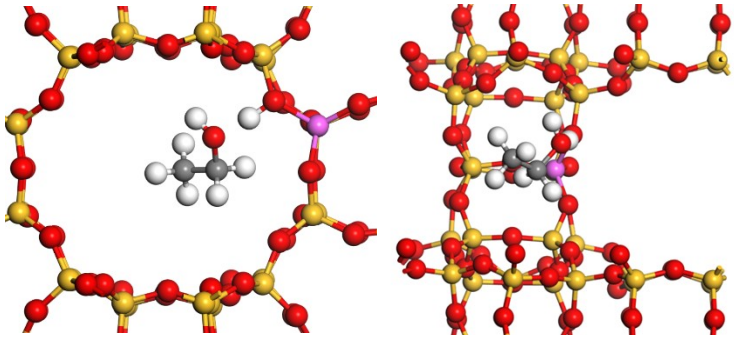


**TS2**

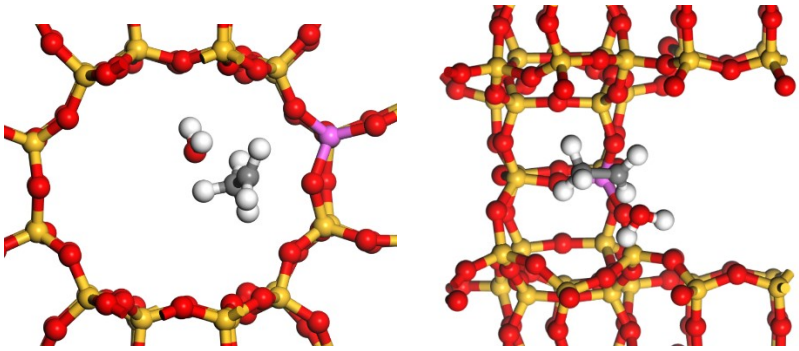


**S5**

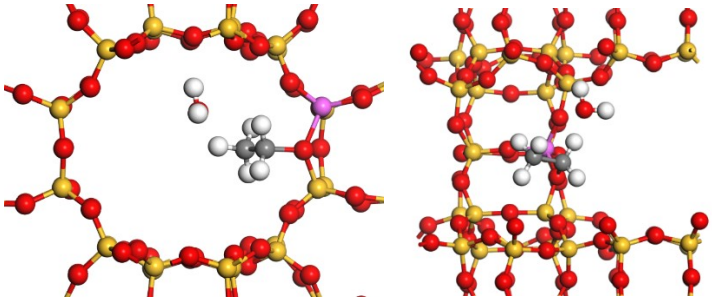
4.4 Configuration of ethanol dehydration on T2 Al-O(H)-Si site (left: top view, right: side view)



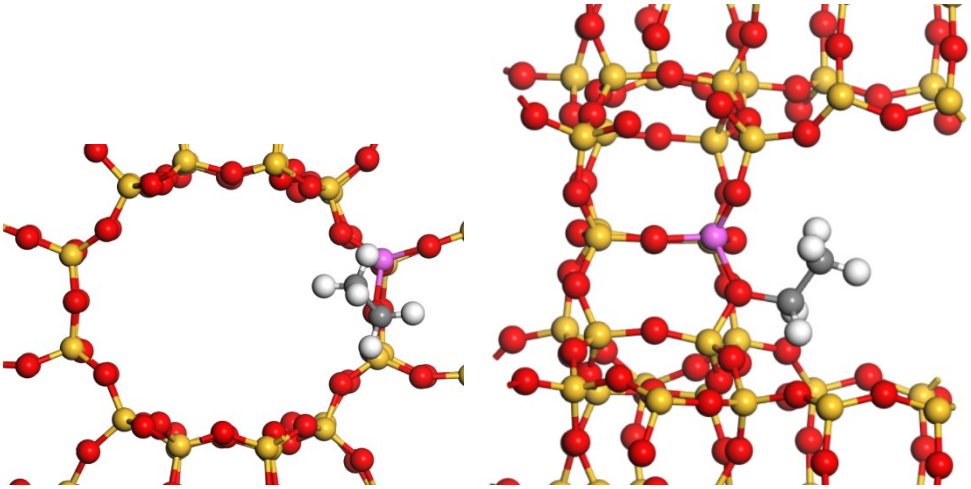
**A2**



**TS3**



**A3**



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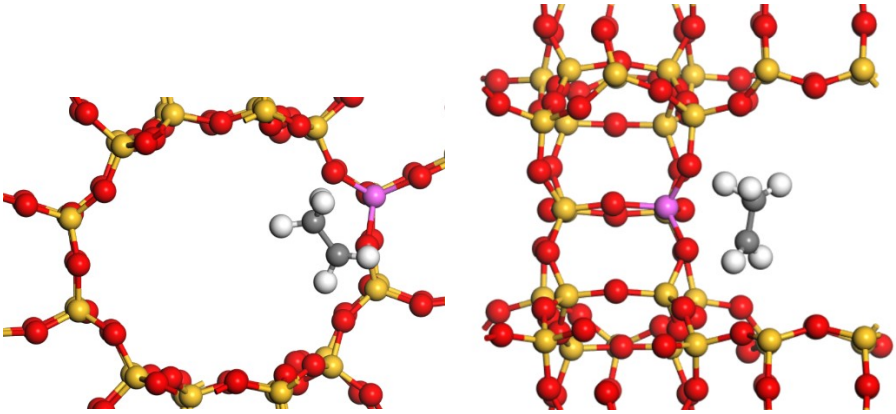
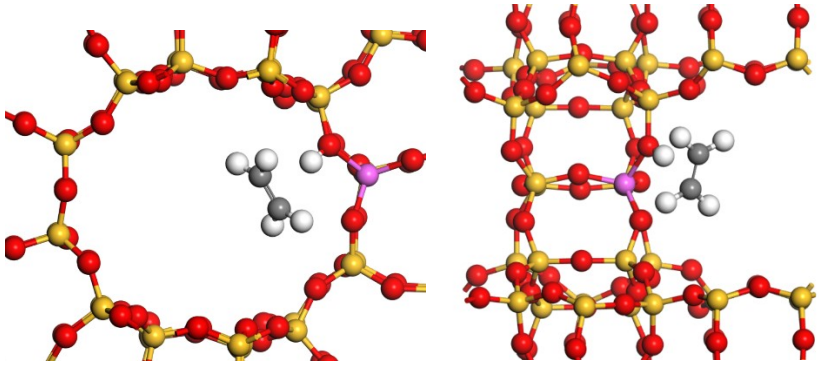


**TS4**



**A5**

## 4.5 Atomic coordinates of key reaction intermediates and transition states

### S2

| | | | |
|---|---|---|---|
| H | 7.40440753 | 10.59132905 | 8.38295071 |
| H | 5.38803940 | 12.53982448 | 9.52122137 |
| H | 4.69367516 | 12.47404096 | 7.64403167 |
| H | 6.24234075 | 11.56033968 | 6.91321265 |
| H | 8.57240259 | 0.39290789 | 7.41457045 |
| H | 9.05234008 | 11.46007197 | 6.75742243 |
| H | 11.00665060 | 0.39393153 | 6.83424885 |
| H | 11.27998163 | 11.58735010 | 7.90874864 |
| H | 10.82148681 | 0.51715021 | 8.60018285 |
| H | 8.35015558 | 12.01015007 | 9.43159012 |
| C | 9.19676280 | 12.12296723 | 7.62329426 |
| C | 10.66154969 | 12.48559499 | 7.78356380 |
| O | 3.96247999 | 8.28627152 | 1.62492386 |
| O | 4.16530245 | 10.39201679 | 26.61897981 |
| O | 2.80079160 | 10.60418638 | 2.23813214 |
| O | 5.45816955 | 10.36548744 | 2.27985796 |
| O | 4.10778564 | 6.29502829 | 26.49452382 |
| O | 2.81958547 | 5.98913102 | 2.18787784 |
| O | 5.46826022 | 6.09184684 | 2.09681277 |
| O | 8.83513841 | 8.26620062 | 1.85954802 |
| O | 10.41092267 | 10.39150635 | 1.56155802 |
| O | 8.05298535 | 10.63290374 | 2.69716842 |
| O | 10.43173468 | 6.16779188 | 1.51178497 |
| O | 8.06294989 | 5.87890927 | 2.65143803 |
| O | 12.04914295 | 8.28892743 | 1.50304794 |
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| O | 0.20282247 | 6.08441997 | 2.62677774 |
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| O | 8.41700627 | 2.08981463 | 13.24047305 |
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| O | 6.95423752 | 2.10577722 | 15.40712611 |
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| O | 7.00153753 | 6.19613783 | 15.49856755 |
| O | 3.69596017 | 4.20483717 | 15.09599169 |
| O | 1.98168146 | 2.16623062 | 15.03522925 |
| O | 4.40520813 | 1.82583303 | 16.00306182 |
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| O | 0.34043398 | 4.27173180 | 14.91540994 |

| | | | |
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| O | 6.15871432 | 6.92685313 | 22.02041122 |
| O | 8.32707318 | 3.61121869 | 21.85095974 |
| O | 10.44056401 | 2.02532555 | 21.52741674 |
| O | 10.71528250 | 4.39308673 | 22.62792009 |
| O | 6.23906128 | 1.98760493 | 21.54738060 |
| O | 5.93066518 | 4.36943968 | 22.64104606 |
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| O | 10.61286220 | 12.26900970 | 22.69310792 |
| O | 6.06487109 | 12.18002468 | 22.54555240 |
| O | 8.43315134 | 8.27726374 | 24.81116025 |
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| O | 9.66408695 | 10.60201358 | 24.55187237 |
| O | 7.01818714 | 10.49574585 | 24.38684436 |
| O | 8.18706513 | 6.40356740 | 0.07737237 |
| O | 9.60682240 | 5.91395376 | 24.53128458 |
| O | 6.95171485 | 6.09797548 | 24.41374030 |
| O | 3.77252312 | 8.40838357 | 24.90798408 |
| O | 2.02973828 | 10.43081170 | 25.02014275 |
| O | 4.41883054 | 10.80440440 | 24.01121974 |
| O | 1.99555613 | 6.42318562 | 24.88960842 |
| O | 4.37380092 | 6.07675508 | 23.84910589 |
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| | | | |
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| O | 12.19053846 | 6.06125515 | 23.94434143 |
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| Si | 6.80517568 | 4.25345625 | 18.40422352 |
| Si | 10.03794415 | 9.04041356 | 18.36575038 |
| Si | 6.85199622 | 9.05319431 | 18.33603319 |
| Si | 10.08274002 | 12.12715257 | 18.44428865 |
| Si | 6.85338818 | 12.13790864 | 18.42332742 |
| Si | 10.90766732 | 6.69963965 | 16.61243652 |
| Si | 2.65282649 | 8.47299924 | 5.07580116 |
| Si | 5.86762600 | 8.43579589 | 5.19095525 |
| Si | 2.53539551 | 3.67667781 | 5.10578368 |
| Si | 5.72640513 | 3.65124287 | 4.96303506 |
| Si | 2.51654075 | 0.59031843 | 5.18140330 |
| Si | 5.75361166 | 0.57374143 | 5.10896766 |
| Si | 1.78386257 | 5.98100763 | 3.27738086 |
| Si | 1.77424538 | 10.94892001 | 3.29356612 |
| Si | 6.65598266 | 6.05414891 | 3.28746348 |
| Si | 10.85806285 | 1.79575752 | 16.56441143 |
| Si | 5.98442426 | 6.70444824 | 16.59412861 |
| Si | 1.77829473 | 1.76399548 | 9.91359952 |
| Si | 6.70710563 | 6.56094962 | 9.92713145 |
| Si | 10.89387424 | 10.88438359 | 23.22159131 |
| Si | 5.96949231 | 5.98543660 | 23.20036475 |
| Si | 5.74804381 | 8.98562088 | 8.22661866 |

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