Supporting Information

Water Molecules Facilitate Hydrogen Release in Anaerobic Oxidation of Methane to Methanol over Cu/Mordenite

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S1. The choice of the spin states of the reaction intermediates.

A number of recent theoretical publications consider the possibility of alternative pathways for the reaction step corresponding to the methane activation depending on the spin state of the original center, with the triplet spin state of the mono(μ-oxo)dicopper species yielding a more energetically favorable pathway. For instance, the work of Li et al., J. Catal. 2016, 338, 305 is the example of the analysis of the mono(μ-oxo)dicopper species in the ZSM-5 zeolite, while the work of Mhyuddin et al., ACS Catal. 2018, 8, 1500, is a corresponding example in the case of CuMOR). We would like to emphasize two crucial points of the above works:

- In both cases above, the initial step of the reaction is the activation of methane in the so-called direct rebound process. There, a direct abstraction of the hydrogen atom occurs over the radical copper oxide species.

- The crossing of spin states from triplet to singlet occurs upon the formation of methanol. Methyl radical and OH ligand are recombined via a transition state to form a low-lying copper/methanol complex in the closed-shell singlet state, indicating the occurrence of a spin inversion from the triplet state to the singlet state before or after that transition state. The possibility of similar spin inversion in copper dimers has also been described by Metz et al. (J. Am. Chem. Soc. 2001, 123, 4938) and Paolucci et al. (Science 2017, 357, 898).

In our original work proposing the possibility of the anaerobic oxidation of methane to methanol (Sushkevich et al., Science 2017, 356, 523, Ref. 16 in the original manuscript), we presented a different methane activation step, consistent with the process of anaerobic oxidation. An important difference in our reaction mechanism is the formation of the Brønsted acid site (BAS) upon activation of methane (which has also been observed experimentally) accompanied by the activation of methane on the copper atom. This leads to the formation of a more mobile Cu···CH_3 fragment, which easily reabsorbs from the copper atom of the active site to the oxygen atom, forming a methoxy species (see the figure below, adopted from Sushkevich et al., Science 2017, 356, 523):

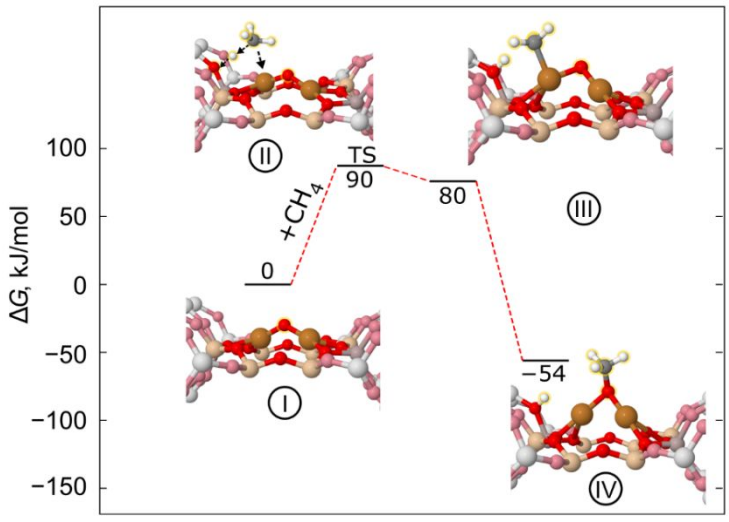


Figure S1. The energetics of the reaction step corresponding to the activation of methane over copper-exchanged mordenite.

Our calculations indicate that such process is favorable, and, most importantly, the suggested model fits the experimental observations. This differs from a direct rebound model used in the above reference.

Notwithstanding these differences, in the current manuscript, on the other hand, we only consider the reaction starting from the Cu(I) methoxy species, where only the spin state of singlet is normally considered. We therefore do not expect the triplet state to be more stable and do not expect any positive differences in the reaction profiles if the spin states are forced to assume a triplet state.

Furthermore, the DFT calculations presented in the current manuscript relied on the automatic optimization of the spin states as implemented in the FHI-aims package. Indeed, the intermediates presented there correspond to the (automatically optimized) singlet spin states.

S2. The location of the copper dimer species.

Copper species could in principle be located both in 8 MR and 12 MR of mordenite. However, the abundant literature on the topic seems to prefer the 8 MR as the host pore for copper species, for instance the dimers and trimers. For example, Grundner et al. (Nat. Commun. 2015, 6, 7546, Ref. 12 in the original manuscript) have recently investigated the siting of the copper oxo species. They have first used different probe molecules (pyridine and *n*-hexane) to determine the acid site distribution in H-MOR, followed by the same analysis of the distribution of residual BAS in Cu-MOR materials after their activation in O_2. The authors concluded that the relatively high concentration of framework Al (65% of the total) in the side pockets is stabilizing Cu clusters there, with the positively charged clusters balancing the charge of two Al sites located in the 8 MR of the side pockets of mordenite. Furthermore, many theoretical studies investigate the copper species located in 8 MR, on the basis of the similarities with the geometry of $[Cu_2(\mu\text{-}O)]^{2+}$ in ZSM-5 zeolite (e.g. Mahyuddin et al., ACS Catal. 2018, 8, 1500, Ref. 24 in the original manuscript). Such location allows the actual reaction to take place in the 12 MR channels of MOR, located perpendicular to the 8 MR, where the space is large enough for the access of methane and methanol molecules.

At the same time, the possibility of the formation of the copper oxo species in the 12 MR has also been investigated, prominently by Zhao et al. (ACS Catal. 2016, 6, 3760). The authors have demonstrated that the CuOCu cluster can either be attached to two T4 sites separated by two T2 sites in the 12 MR or to two T3 sites separated by two T1 sites at the intersection of the side pocket within the 8MR. The authors show that the free energies of the C-H bond dissociation are in a narrow range from 43 to 76 kJ/mol, except for that occurring on in the 8MR, as the side pocket is too small to fit the CH_3 radical.

As indicated above, however, in our case the reactants are assumed to be located above the 8 MR pore in the space of the 12 MR channel, and not in the side pocket. An example of this can be seen below:

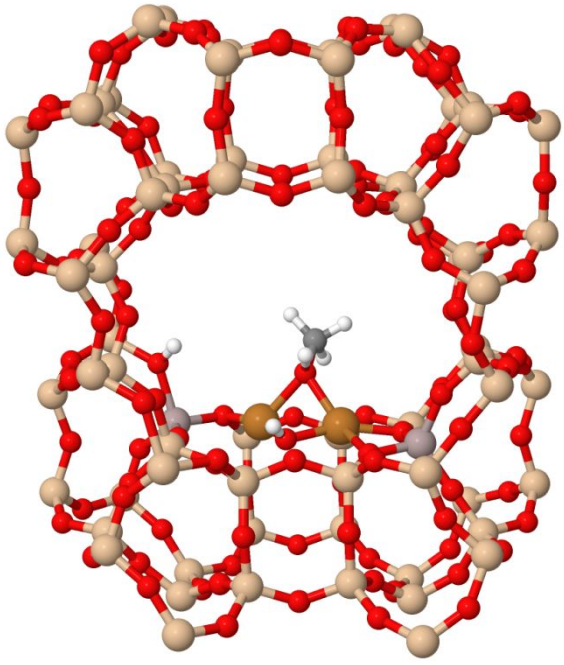


Figure S2. The 12 MR channel of mordenite, in which space the reaction takes place.

Clearly, due to the size of the main 12 MR channel, the reactants are not constrained in their movement.

Moreover, we have previously compared a "conventional" mono(μ-oxo)dicopper species located in the 8 MR pore of mordenite with a system of two monomers in the larger 12 MR pore that can interact with each other, and have shown that their behavior is quite similar (Sushkevich et al., Angew. Chem. Int. Ed. 2018, 57, 8906, Ref. 32 in the original manuscript).

Notwithstanding, following the suggestion by the referee, we have compared the energies of the methanol activation within our model and the various models in the 12 MR, as described by Zhao et al. Here we compare the energetics of the first C-H bond activation of the adsorbed methane molecule on the mono(μ-oxo)dicopper center in the 8 MR of mordenite (as described in our original work on anaerobic oxidation, Sushkevich et al., Science 2017, 356, 523, Ref. 16 in the original manuscript) with the same process for our model of paired monomers in the 12 MR, and the data from Zhao et al.:

Reference	**Pore size**	**C-H dissociation step free energy, kJ/mol**	**Free energy barrier, kJ/mol**
Ref. 16	8 MR	80	90
Ref. 32	12 MR	79	87
Zhao et al.	12 MR	43–76	63–99

As can be seen from the table above, our numbers are generally in the range reported by Zhao et al.

S3. Ensuring the robustness of the molecular dynamic simulations.

To ensure that the system does not get trapped in one possible region of the configurational space, we tried to let the system assume the features typical for higher temperature simulations, by applying the replica exchange algorithm (Phys. Rev. Lett. 1986, 57, 2607; Phys. Chem. Chem. Phys. 2005, 7, 3910). As a test, we re-ran the simulation corresponding to the transition between the intermediate I and intermediate II, by running 11 simulations concurrently, ranging from the temperatures of 423 K to 523 K, with the 10 K temperature step between the replicas. Swaps between adjacent temperatures were attempted every 10 ps, with the exchange probability given by

$$P = \min\left\{1, \exp\left(-\frac{(V_j - V_i)(T_j - T_i)}{T_i T_j k_{\mathrm{B}}}\right)\right\},$$

where V_i and V_j , and T_i and T_j are potential energies and temperatures of two adjacent replicas, respectively, and k_{B} is the Boltzmann constant.

We have found that, compared to the simulations carried out at a constant temperature of 473 K, no qualitatively new chemically relevant configurations were found, as can be seen from the distribution of energy shifts compared by the higher temperature replicas compared to the lowest temperature one:

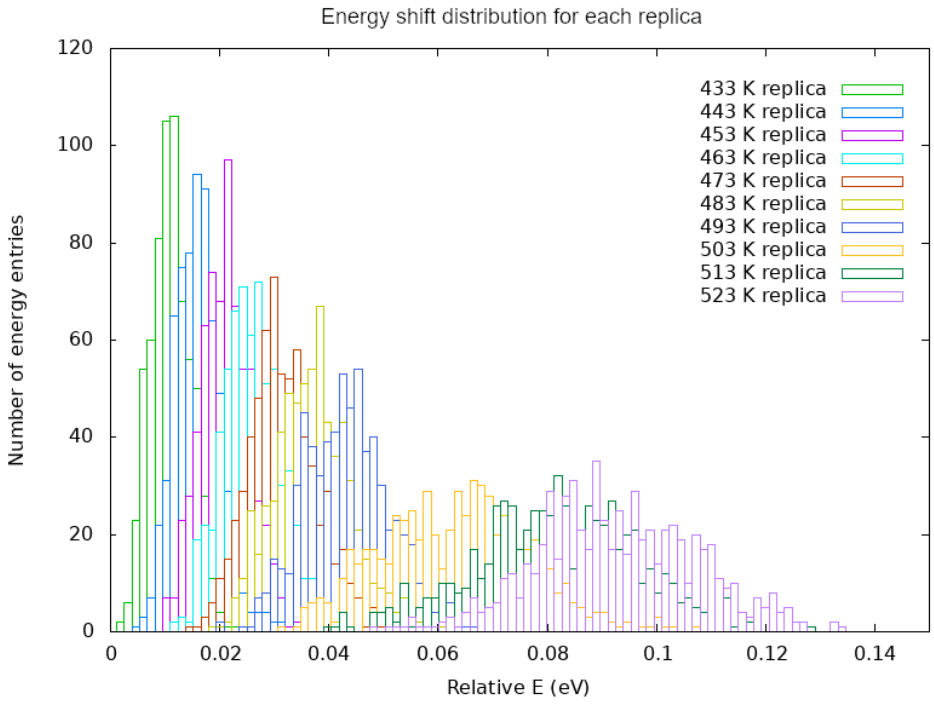
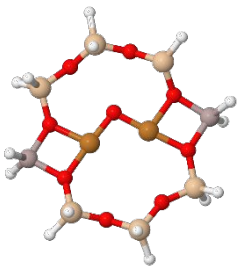
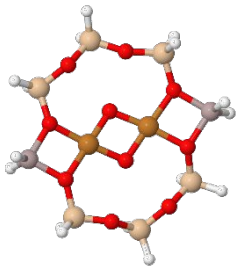
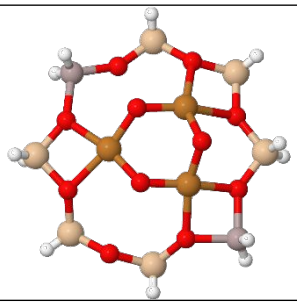


Figure S3. Histogram of the energy distribution of replicas used in the molecular dynamics simulation.

As can be seen from the figure above, a typical energy shift distribution range is quite narrow at about 0.12 eV (~12 kJ/mol), illustrating that the temperature of 473 K must have already sampled most of the relevant configurations.

S4. Comparison of PBE0 and CCSD calculated electron binding energies.

Table S1. Comparison of some of the example XPS Cu $2p_{3/2}$ binding energies of CuMOR calculated at different levels of theory.

Structure	Cluster configuration	Cu $2p_{3/2}$ BE, eV	
		Periodic PBE0	Cluster CCSD
MOR: mono(μ-oxo) dicopper		934.3	934.5
MOR: bis(μ-oxo) dicopper		936.1	936.1
MOR: tricopper		934.8 & 935.9	934.9 & 935.7

S5. Important geometrical parameters of all reaction intermediates.

Table S2. Some of the geometric parameters of the identified reaction intermediates.

Intermediate	Name	Cu-O bond length, Å	Cu-Cu bond length, Å	Cu-O-Cu angle, °
I	methoxy	1.85	2.82	90.3
I’	methoxy with adsorbed water	1.88	2.73	93.5
TS1	TS1	2.02	2.35	70.7
II	hydroxy	1.84	2.72	95.4
II’	hydroxy with adsorbed water	1.86	2.84	99.2
TS2	TS2	1.91	2.98	111.9
III	hydride with adsorbed methanol	1.85	2.49	85.1
IV	hydride	1.90	2.55	85.3
IV’	hydride with adsorbed water	1.89	2.55	85.2
TS3	TS3	2.01	3.02	116.6
V	mono(μ-oxo) with adsorbed water	1.75	2.75	103.3
TS4	TS4	2.02	3.05	105.3
VI	dihydroxo	1.89	2.99	104.8

S6. Analysis of the configuration of the [Cu–H] intermediate

[Cu–H] species act as unstable transition state configurations in all steps of the reaction but one, that of the structure IV in Fig. 1 in the main text, formed upon overcoming the largest energy barrier in the entire reaction pathway. Nevertheless, this is a locally stable intermediate, as evidenced by the absence of imaginary frequencies in the calculated vibrational spectrum. This is in line with experimental evidence suggesting the existence of copper hydride species and their catalytic activity (Refs. 44–46 in the main text). To get insight into the nature of chemical bonding of this species and its chemical reactivity, we look at the electronic density distribution of its highest occupied molecular orbital (HOMO).

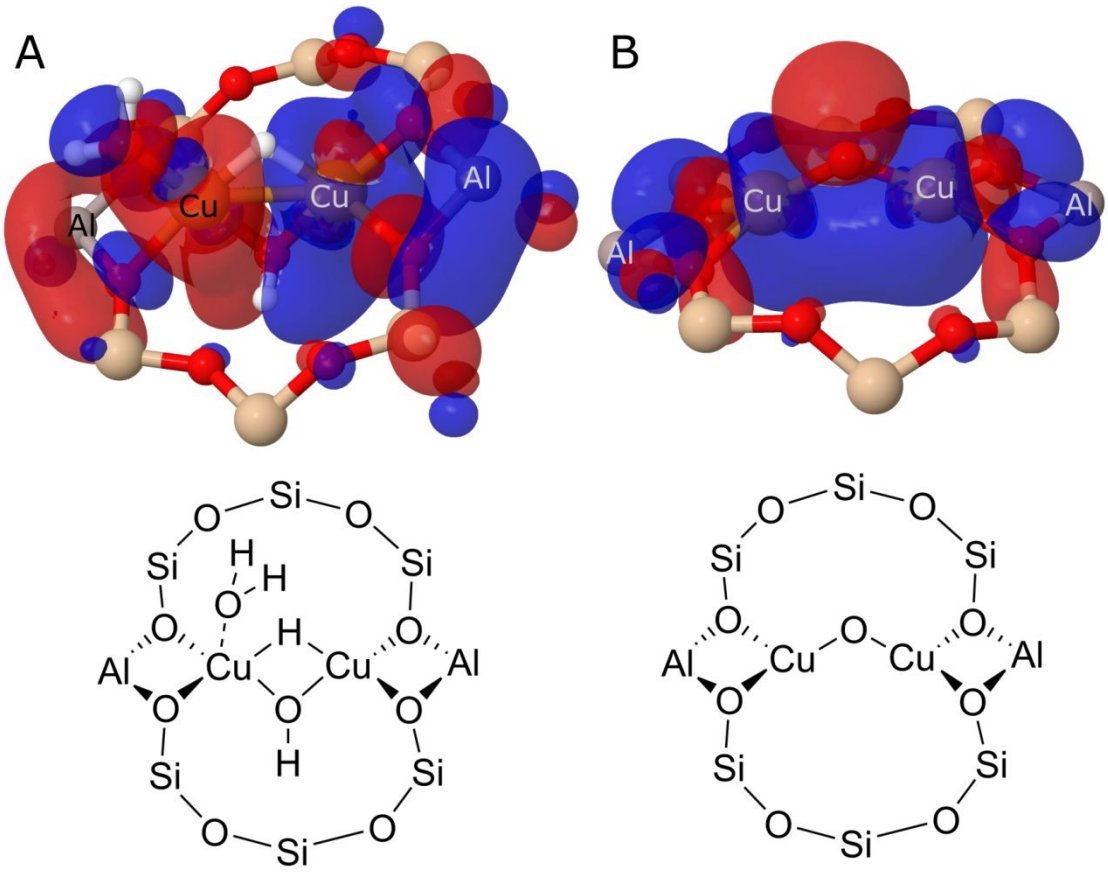


Figure S4. Comparison of the HOMO orbitals of A) the [Cu–H] intermediate IV (see Fig. 1 in the main text) and B) the original mono(μ-oxo)dicopper active center. The 3D isosurface is plotted at 0.02 e/Å^3.

Analysis of the HOMO of the [Cu–H] intermediate reveals that both the hydride and the hydroxy group are located between two lobes of electronic density centered around one of the two copper atoms (panel A in the figure above). This is in contrast with the original mono(μ-oxo)dicopper core, where both copper atoms are connected (panel B in the figure above). The main difference between the nature of the formed bond in both cases is the availability of the oxygen atom between the two copper atoms to facilitate the bonding. While in the case of a mono(μ-oxo)dicopper species both valences of oxygen is used to bind copper atoms, the [Cu–H] intermediate features a hydroxy group from the previously adsorbed water molecule. As a result, such a structure is less strongly bonded, suggesting an easy hydrogen abstraction during the next

step. Additionally aided by the fact that the Cu–Cu distance in such a [Cu–H] intermediate is only 2.55 Å, i.e. copper atoms are located much closer than in the original mono(μ-oxo) dicopper core (3.12 Å), such a configuration makes the shift of both hydrogen atoms towards one of the copper atoms feasible, thus facilitating energetically favourable route of the molecular hydrogen formation.

S7. Analysis of the water content in the zeolite under reaction conditions

The exact amount of consumed water under experimental conditions is of utmost interest. We conducted a quick analysis of the influence of the pressure of water on the ratio of concentrations of adsorbed water and the total amount of active sites at the reaction temperature of 473 K, according to the classical Langmuir model expressed as follows:

$$C_{\text{water}} = C_{\text{sites}} \cdot \frac{k \cdot P_{\text{water}}}{1 + k \cdot P_{\text{water}}} \quad (1)$$

where C_{water} is the concentration of the adsorbed water, C_{sites} is the total concentration of the metal sites, k is the equilibrium constant of the adsorption, and P_{water} is the pressure of gaseous water. The equilibrium constant can be expressed in terms of the enthalpic and entropic contributions of the corresponding reaction step:

$$\ln k = -\frac{\Delta H}{RT} + \frac{\Delta S}{R} \quad (2)$$

where k is the equilibrium constant of the adsorption, ΔH and ΔS are the enthalpy and the entropy of the step at given conditions, T – temperature and R – universal gas constant.

As an example, we plotted an adsorption isotherm diagram for the case adsorption of three water molecules on the methoxy species formed at the mono(μ-oxo)dicopper site of the copper exchanged mordenite (corresponding to the cyan line, structure I', in Figure 2 of the current version of the manuscript). Please note that three water molecules is an optimal amount needed to facilitate the proposed mechanism, with the minimum number of water molecules actually participating in the reaction being two.

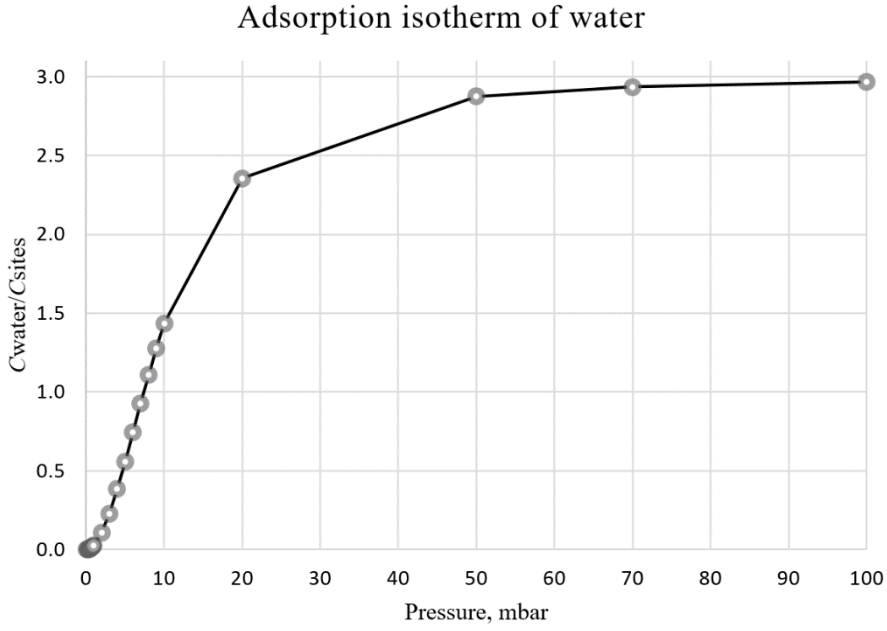


Figure S5. Adsorption isotherm of three water molecules on the methoxy species formed at the mono(μ-oxo)dicopper site of the copper exchanged mordenite.

As can be seen from the plot above, the saturation of the active sites with two water molecules is already achieved at the water pressures as low as ~16 mbar. The actual experimental conditions

imply the purge of water vapour in helium through the system at the pressure of 1 bar, with a 2.6 vol% of water (i.e. 26 mbar of water), thus making the presence of two water molecules per active site of the zeolite highly probable.

It should be emphasized, however, that the estimation above is oversimplified. Firstly, it only considers one adsorption situation, and does not account for mixed adsorption configurations, such as, for example, a mixture of singly/doubly/triply occupied sites. Secondly, the model only assumes the presence of mono(μ-oxo)dicopper sites, and does not take into account multiple possible Cu_xO_y species. Most importantly, adsorption of water is not only possible on copper active sites, but also on the zeolite framework itself. This dramatically increases the number of easily assessable water molecules, already confined within the vicinity of the active sites, and readily available for the reaction.

Notwithstanding, there is no doubt that adsorption of several water molecules per active site is experimentally feasible. Zeolites in general, including metal exchanged zeolites, are known to have a very high water adsorption capacity (see e.g. E.-P. Ng et al., Micropor. Mesopor. Mat. 2008, 114, 1-26). For instance, in the above paper by Nan et al. (Ind. Eng. Chem. Res. 2017, 56, 8095–8102), the maximum observed water adsorption capacity of silver-exchanged mordenite was reported to be as high as 20 wt. %. For comparison, adsorption of two water molecules per unit cell of our sample would be equivalent to only around 1.2 wt. %.

S8. Cartesian coordinates and lattice parameters of all identified intermediates and transition states in Fig. 1.

Intermediate I

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lattice_vector 0.00000000 20.53400000 0.00000000
lattice_vector 0.00000000 0.00000000 7.54200000

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Intermediate I'

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