Electronic Supporting Information for<br>Methane to Methanol over Copper Mordenite: Yield Improvement Through Multiple Cycles and Different Synthesis Techniques<br>by<br>Selmi E. Bozbag ${ }^{1,2,3}$, Evalyn Mae C. Alayon ${ }^{2,3}$, Jan Pecháček ${ }^{2}$, Maarten Nachtegaal ${ }^{1}$, Marco Ranocchiari ${ }^{1}$, Jeroen A. van Bokhoven ${ }^{1,2, *}$<br>${ }^{1}$ Paul Scherrer Institute, Villigen, CH-5232 Switzerland<br>${ }^{2}$ ETH Zurich, Wolfgang-Pauli-Strasse 10, CH-8093 Zurich, Switzerland<br>${ }^{3}$ : Authors contributed equally.<br>*: Corresponding author; e-mail: jeroen.vanbokhoven@chem.ethz.ch; Tel.: + 41446325542

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## 1. Catalytic Activity



Figure S1 Mass spectrometer-detected signals of $\mathrm{H}_{2} \mathrm{O}(\mathrm{m} / \mathrm{z}=18)$, and methanol $(\mathrm{m} / \mathrm{z}=31)$ during the treatment of wet He at $200^{\circ} \mathrm{C}$ after methane interaction of $\mathrm{CuMOR}_{\mathrm{S}}$ during $2^{\text {nd }}$ cycle.

## 2. $\mathbf{N}_{2}$ Adsorption

Table S1 BET Number of the materials used in this study

| Material | BET surface area <br> $\left[\mathrm{m}^{2} / \mathrm{g}\right]$ |
| :---: | :---: |
| Na-MOR | 411 |
| H-MOR | 464 |
| CuMOR $_{\mathrm{A}}$ | 386 |
| CuMOR | 410 |
| CuMOR $_{\mathrm{S}}$, after 2 cycles of R1 | 328 |
| CuMOR $_{\mathrm{S}}$, after 8 cycles of R1 | 202 |

3. XAS spectra taken during in situ synthesis of $\mathrm{Cu}-\mathrm{MOR}_{\mathrm{S}}$


Figure S2 XANES and FT EXAFS spectra taken during in situ synthesis of $\mathrm{Cu}-\mathrm{MOR}$ by heating of CuCl and $\mathrm{H}-\mathrm{MOR}$


Figure ES3-2. XANES spectra of standard copper compounds

## 4.Linear Combination Fitting



Figure S4 XANES spectra of standard copper compounds used in the LCF.


Figure S5 XANES Spectra taken during $\mathrm{O}_{2}$ activation ( $\mathrm{a}, \mathrm{c}, \mathrm{e}$ ) and $\mathrm{CH}_{4}$ reaction (b, d, f) of $\mathrm{Cu}-\mathrm{MOR}_{\mathrm{S}}$ at the corresponding cycle with the linear combination fit, its components and the residual.


Figure S6 XANES Spectra taken during $\mathrm{O}_{2}$ activation ( $\mathrm{a}, \mathrm{c}, \mathrm{e}$ ) and $\mathrm{CH}_{4}$ reaction (b, d, f) of $\mathrm{Cu}-\mathrm{MOR}_{\mathrm{A}}$ at the corresponding cycle with the linear combination fit, its components and the residual.

