## **Supplementary Information**

## Influence of Topology and Brønsted Acid Site Presence on Methanol Diffusion in Zeolites Beta and MFI

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The supplementary information contains plots of contact auto-correlation function for the H-Beta and H-MFI models used for calculating the residence time of methanol molecules at the Brønsted acid site are also give.



**Figure S1**. Plots of contact auto-correlation function for the H-Beta (a) 2 mpuc with (b) 4 mpuc and H-MFI (c) 3 mpuc with (d) 5 mpuc models calculating the residence time of methanol molecules at the Brønsted acid site. The curves represent the exponential fitting for the simulation data.