Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Computational Understanding of Na-LTA for Ethanol−Water Separation

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1. Barrier for H_2O passing through the 6MR.

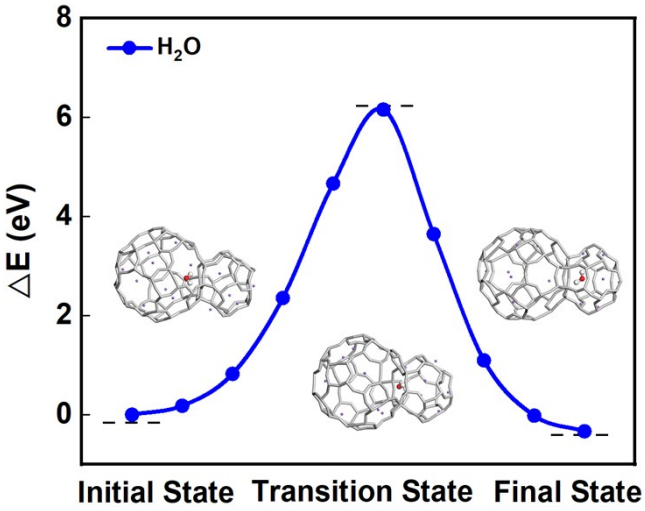

Fig. S1. Energy barriers for H_2O crossing the 6MR without Na^+ located in 6MR.

This calculation was completed using the CINEB[1]method, and from it, we can observe that the energy barrier for a single water molecule to pass through a six-membered ring exceeds 6 eV.

2. Calculations based on the volumetric density for confirm the loading.

By using Materials Studio, the free volume of the framework model was determined as 790.93 Å3, with a probe molecule of 1.5 Å in diameter. The highest loading of water is estimated to be:$V_{free} = 790.93\ \text{Å}^3$with a probe molecule of 1.5 Å in diameter. The highest loading of water is estimated to be:

$$N_{H_2O} = N_A * \frac{\rho_{H_2O} V_{free}}{M_{H2O}} = \frac{1\ g/\ cm^3 * 790.93\ \text{Å}^3/cell}{18.0\ g/mol} * 6.022 * 10^{23}/mol = 26\ H_2O/cell$$

Since the diameter of the probe molecule is underestimated, we studied systems with slightly lower loading (24 water molecules per cell) to facilitate the motion of water. Furthermore, two other different water uptakes (16 and 32 molecules per cell) were investigated to understand the effect of varying upload. Similarly, the loading of ethanol molecules was determined.

References

1. G. Henkelman, B P. Uberuaga, H. Jónsson, *The Journal of chemical physics*, 2000, **113**: 9901-9904.