

Enhancing diffusion selectivities by molecular traffic control in FER-type zeolites

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Detailed understanding how molecular transport in nanoporous materials is influenced by various features of the host structure can provide new insights towards further optimization of their performance in technical applications, such as catalysis, separations, molecular storage and sensing [1,2]. We present a study of the diffusivity of small alkanes and alcohols in siliceous ferrierite [3]. A surprisingly high difference in the diffusivities of methanol and ethanol has been observed ($D_{MeOH}/D_{EtOH} \approx 25,000$). This difference most likely results from an interplay of two phenomena, which have been recently discussed as options to manipulate mixture diffusion, viz. molecular traffic control and clustering effects. The major conclusion can be summarized in two points: (i) molecular traffic control effects can be facilitated by molecular clustering and (ii) their combination provides a new option for enhancing diffusion selectivities and, thus, for further optimizing the use of nanoporous crystalline materials in technical applications.

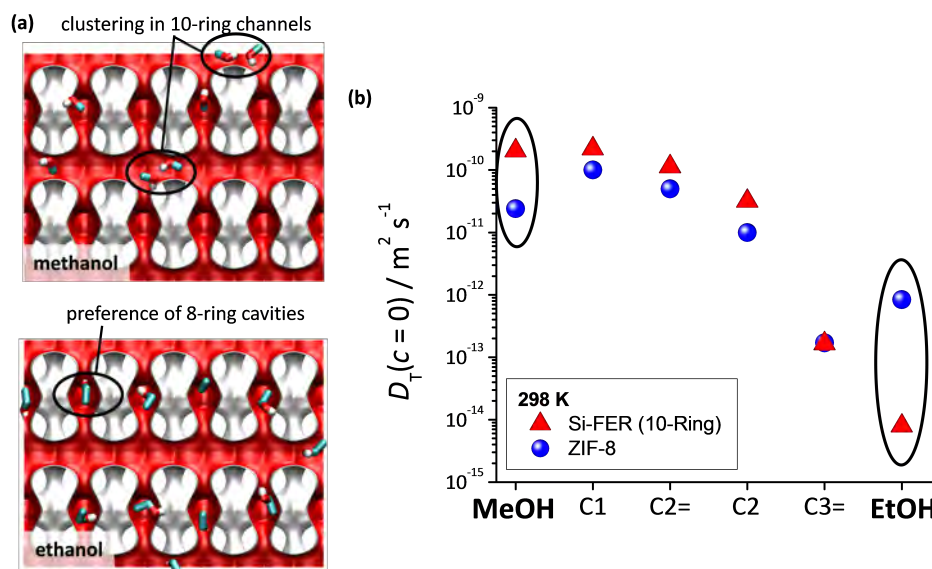


Figure 1: (a) CBMC snapshots showing the location of methanol and ethanol in Si-FER at a loading of 2 molec/uc at 298 K. (b) Comparison of the zero-loading diffusivities for various small molecules in Si-FER (triangles) and ZIF-8 (spheres).

References

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