

## **Diffusion in Zeolites – Applications and Challenges**

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Diffusion of guest molecules under confinement of zeolites shows many interesting properties due to guest-host interactions. This talk explores some of the applications and challenges relating to the diffusion of guest molecules in zeolites using molecular dynamics simulations.

Comparative diffusion of hexane isomers inside zeolite Y is used for separation of the isomer mixtures in petroleum industries. The order of exit of different isomers from a zeolite Y column depends on the order of their diffusivities. It is seen that the self-diffusivities of the isomers exhibit an anomalous dependence on their molecular diameter. This anomalous dependence of diffusivity is in excellent agreement with the predictions of Levitation Effect (LE). Also, this order can be controlled by varying the temperature to achieve kinetic separation of these mixtures.

Meanwhile, the diffusivity values,  $D$ , measured using methods like uptake or PFG-NMR are often smaller by several orders of magnitude than those measured using methods like QENS or MD simulations. To understand the underlying reason for this reduction in  $D$ , molecular dynamics simulations of guest molecules have been carried out in zeolite systems where an inter-crystalline space is introduced. It is seen that the  $D$  in these systems are significantly altered by the presence of the inter-crystalline space and the value is smaller compared to the other axes, which reduces the total effective  $D$  when compared to a purely intra-crystalline diffusion.