

# Molecular simulation of alkane and alkene diffusion in nanoporous membranes to allow for an energy-efficient separation.

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In context of the current energy crisis, improving the efficiency of highly energy consuming processes is more relevant than ever. One of the most energy-intensive chemical processes is the separation of alkanes and alkenes, which accounts for 0.3% of the world's energy consumption (Stephenson, 2019). The most common way to separate alkanes and alkenes is via cryogenic distillation. However, a significant improvement in energy retention could be achieved by applying room temperature sieving of the molecules. For this purpose, membranes made out of nanoporous crystalline materials known as zeolitic imidazolate frameworks (ZIFs) will be investigated for their high selectivity in separation of ethane from ethene (C2) and propane from propene (C3) species at room temperature.

In this work, the nature of C2/C3 separation by means of a diffusion analysis in ZIF-8 is investigated. To examine the diffusion behavior of individual molecules, computer simulations that solve Newton's equations of motion on a molecular level using classical potentials for the inter- and intramolecular interactions are performed. The diffusion path of an alkane or alkene molecule through ZIF-8 is modeled with advanced MD simulation techniques. The result of this simulation is the thermodynamic free energy and its enthalpic and entropic contributions as a function of the progress along the diffusion pathway. From this free energy profile a diffusion rate can be determined. This means that the structure of the molecular system and the diffusion rate of guest molecules can be correlated. By applying this modeling procedure for a number of different host materials and guest species, more thorough insight into the effects of different structural elements on hydrocarbon diffusion can be obtained, which is an essential element in the design of new material for a highly efficient separation of alkanes and alkenes.