Pore Size or Geometry: Which Determines the Shape and Inverse-Shape Selective Adsorption of Alkane Isomers?

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The adsorption of pure pentane (C5) isomers and their ternary mixtures are simulated in a series of carbon nanoslits. With decreased nanoslit pore size, first shape selective adsorption occurs on the order of nC5 > iC5 > neoC5, due to the configurational entropy effect, then inverse-shape selective adsorption occurs in the order of nC5 < iC5 < neoC5, due to the length entropy effect, and, finally, no adsorption occurs. The entropy effects are found to lead to a large adsorptive separation of the C5 isomers from their mixtures. Similar behavior has been observed in the simulation of C5 adsorption in carbon nanotubes with identical pore sizes. These results reveal that pore size, rather than geometry, determines the shape and inverse-shape selective adsorption of alkane isomers in nanopores.